

**On Plastic Flow in Solids with Interfaces**

by

Anurag Gupta

B.Tech. (Indian Institute of Technology, Roorkee) 2002  
M.S. (University of California, Berkeley) 2003

A dissertation submitted in partial satisfaction of the  
requirements for the degree of  
Doctor of Philosophy

in

Engineering-Mechanical Engineering

in the

GRADUATE DIVISION

of the

UNIVERSITY OF CALIFORNIA, BERKELEY

Committee in charge:

Professor David J. Steigmann, Chair

Professor George C. Johnson

Professor Jon Wilkening

Fall 2008

The dissertation of Anurag Gupta is approved:

---

Chair

Date

---

Date

---

Date

University of California, Berkeley

Fall 2008

**On Plastic Flow in Solids with Interfaces**

Copyright 2008

by

Anurag Gupta

## Abstract

On Plastic Flow in Solids with Interfaces

by

Anurag Gupta

Doctor of Philosophy in Engineering-Mechanical Engineering

University of California, Berkeley

Professor David J. Steigmann, Chair

The aim of this thesis is two fold. First, we construct a framework for a general theory of anisotropic thermoplasticity, which encompasses previously established models and several seemingly independent lines of research. The theory is based on the two laws of thermodynamics and basic invariance requirements. Invariance is imposed under arbitrary changes in the reference configuration, frame indifference, and material symmetry. The interplay between constitutive assumptions and kinematics is, in particular, emphasized. The classical models of plastic flow are deduced under additional assumptions and a few explicit results are obtained for materials with cubic symmetry. Second, we study interfaces in a plastically deforming solid. The interfaces are assumed to be in the form of waves (shock waves and acceleration waves), grain boundaries, and phase boundaries. The concept of surface dislocations is rigorously established and the governing equations for the dynamics of shock waves and acceleration waves are obtained. In addition, simple examples demon-

strating the behavior of these plastic waves are considered. Finally a theory, where the interface itself contributes energetically, is constructed. The resulting formulation provides us with a basis to study the coupling between grain boundary migration and accompanying plastic flow.

---

Professor David J. Steigmann  
Dissertation Committee Chair

To my parents

I am standing at the threshold about to enter a room. It is a complicated business. In the first place I must shove against an atmosphere pressing with a force of fourteen pounds on every square inch of my body. I must make sure of landing on a plank traveling at twenty miles a second round the sun - a fraction of a second too early or too late, the plank would be miles away. I must do this whilst hanging from a round planet head outward into space, and with a wind of aether blowing at no one knows how many miles a second through every interstice of my body. The plank has no solidity of substance. To step on it is like stepping on a swarm of flies. Shall I not slip through? No, if I make the venture one of the flies hits me and gives a boost up again; I fall again and am knocked upwards by another fly; and so on. I may hope that the net result will be that I remain about steady; but if unfortunately I should slip through the floor or be boosted too violently up to the ceiling, the occurrence would be, not a violation of the laws of Nature, but a rare coincidence. These are some of the minor difficulties. I ought really to look at the problem four-dimensionally as concerning the intersection of my world-line with that of the plank. Then again it is necessary to determine in which direction the entropy of the world is increasing in order to make sure that my passage over the threshold is an entrance, not an exit.

Verily, it is easier for a camel to pass through the eye of a needle than for a scientific man to pass through a door. And whether the door be barn door or church door it might be wiser that he should consent to be an ordinary man and walk in rather than wait till all the difficulties involved in a really scientific ingress are resolved.

A. S. Eddington. In *The Nature of the Physical World*, Cambridge, page 342, 1932.

# Contents

<b>1</b>	<b>Introduction</b>	<b>1</b>
1.1	Plasticity: the phenomenon . . . . .	2
1.2	Plasticity as a thermodynamically irreversible process . . . . .	8
1.3	Continuum theories of plasticity . . . . .	11
1.4	Overview of the thesis . . . . .	15
<b>2</b>	<b>Continuum Mechanics</b>	<b>20</b>
2.1	Kinematics . . . . .	23
2.1.1	Body, configurations and motion . . . . .	23
2.1.2	Derivatives . . . . .	26
2.1.3	Deformation gradient . . . . .	28
2.1.4	Singular surfaces . . . . .	37
2.2	Balance laws and dissipation . . . . .	47
2.2.1	Integral theorems . . . . .	47
2.2.2	Balance laws and jump conditions . . . . .	55
2.2.3	Clausius-Duhem inequality . . . . .	69
<b>3</b>	<b>A Continuum Theory of Plastic Deformation</b>	<b>74</b>
3.1	Unloading elastic bodies to zero stress . . . . .	77
3.2	Deformation and incompatibility . . . . .	85
3.2.1	Dislocation density . . . . .	86
3.2.2	Single dislocations . . . . .	88
3.2.3	Geometrically necessary and statistically stored dislocations . . . . .	91
3.3	Invariance under compatible changes in the reference configuration . . . . .	95
3.4	Thermodynamics of plastic flow . . . . .	100
3.4.1	State variables and constitutive assumptions . . . . .	100
3.4.2	Dissipation . . . . .	103
3.4.3	Isothermal and adiabatic processes . . . . .	106
3.5	Superposed rigid motions . . . . .	108
3.6	Material symmetry . . . . .	112
3.7	Flow and yield . . . . .	117
3.7.1	Flow rule . . . . .	117



3.7.2	Yield criteria . . . . .	126
3.8	Remarks . . . . .	127
<b>4</b>	<b>Plasticity with Small Elastic Strains and Elastic Rigidity</b>	<b>133</b>
4.1	Ilyushin's postulate . . . . .	135
4.2	Small elastic strains . . . . .	141
4.2.1	Preliminaries . . . . .	142
4.2.2	Associated flow rules . . . . .	145
4.3	Elastically rigid, perfectly plastic material . . . . .	151
4.3.1	Preliminaries . . . . .	151
4.3.2	Example of a yield criterion and a flow rule . . . . .	157
4.3.3	Lüders bands . . . . .	159
<b>5</b>	<b>Surface Dislocations and Plastic Waves</b>	<b>164</b>
5.1	Dislocation distribution at the interface . . . . .	166
5.1.1	Surface dislocation density . . . . .	167
5.1.2	True surface dislocation density . . . . .	174
5.1.3	Jump in the bulk dislocation density . . . . .	179
5.2	Shock waves . . . . .	184
5.2.1	Elastic shock wave . . . . .	187
5.2.2	Plastic shock wave . . . . .	191
5.2.3	Shock wave as a dislocation wall . . . . .	194
5.3	Acceleration waves . . . . .	203
5.3.1	Elastic acceleration wave . . . . .	210
5.3.2	Plastic acceleration wave . . . . .	214
<b>6</b>	<b>Interfacial Plastic Flow</b>	<b>226</b>
6.1	Invariance under compatible changes in the reference configuration . . . . .	228
6.2	Thermodynamics: dissipation inequality . . . . .	233
	<b>Bibliography</b>	<b>242</b>

## Acknowledgments

This thesis represents my academic progress of almost twenty-five years of formal learning. I have been highly fortunate to live among people who encouraged not only intellectual freedom, but also a persisting love for knowledge. A comprehensive acknowledgment would result in a volume far exceeding the size of the present thesis. Subsiding under such a practical limitation, I would attempt to thank only a few who have influenced me and my work in the past six years of my doctoral study.

First and foremost I thank Professor David Steigmann, whose research and teaching methodologies have provided new directions to my intellect. His unaffected disposition, be it personal or scientific, has been always a source of inspiration to me. I would like to attribute the merit, if any, in my thesis to him. All the shortcomings are, of course, mine.

Berkeley provided me with an opportunity to experience learning through excellent course work across many scientific disciplines. In particular, I am indebted to Professor Steigmann for his courses on Solid Mechanics, to Professors Petr Hořava and Edgar Knobloch for their courses on Nonlinear Dynamics, and to Professors Grigory Barenblatt, Alexandre Chorin, and Donald Sarason for their courses on Mathematics.

Special thanks are due to Professor Xanthippi Markenscoff, who provided much support towards my academic progress during the entire doctoral study. I deeply cherish my long standing collaboration with her. A great source of intellectual stimulation came from my interactions with Dr. James Stölken, who enthusiastically encouraged my ideas in research and patiently taught me many concepts from experimental material science. I will be forever grateful for his encouragement and mentorship.

My graduate studies at Berkeley were supported through several teaching assistant positions in the first four years and through the Lawrence fellowship from Lawrence Livermore National Laboratory (LLNL) in the last two years. I would like to acknowledge the support, through the teaching positions, offered by the departments of Civil and Environmental Engineering, Mechanical Engineering, and Statistics. I am very thankful to LLNL whose fellowship provided me with both academic and financial freedom.

I would like to thank Professor Steigmann and Dr. Stölken for perusing my thesis and offering their constructive criticism. I am also grateful to Professors George Johnson and Jon Wilkening for agreeing to be on my dissertation committee and for meeting me several times to discuss my thesis. I am thankful to Jyothi Krishnan, who carefully read the introduction chapter and helped me with many corrections, and Christian Linder, who provided several comments on an earlier version of Chapter 2.

My life at Berkeley was further enriched by several friendships that I have enjoyed during the past few years. With Ambuj, who was my apartment-mate for more than five years, I learnt to live independently and prepare the base for a life long journey into the world. We share, among many things, our deep love for culture and art. With Kranthi, I have relished long hours of discussions on topics ranging from thermodynamics to Indian classical music, mostly over tea. With Vishnu and Marghoob, I have enjoyed many fine evenings, dinners, and several hours of squash. A few of other friends, who made a difference to my life at Berkeley include Ashutosh, Christian, Jyothi, Matt, Roger, Saurabh, Steven, Tsuyoshi, and Ushnish.

The acknowledgments will be incomplete without the mention of people who, al-

though not being physically present in Berkeley, provided me with love and kind support from distant places. My parents, to whom I dedicate this thesis, have always nurtured the right values in me and provided me with the strength to lead a responsible life. I would be forever indebted to their patience and trust. My sister Priti and my brother-in-law Rajeev have been a constant source of affection. Many old time friends: Chaitanya, Gita, Shilpi, and Sumit, have always remained close with their warmth and cheerfulness.

# Chapter 1

## Introduction

A solid body is said to deform *plastically* if it undergoes permanent structural changes during the deformation process. The solid acquires a permanent change in its structure if, on restoring the external environment (under which the deformation process has taken place) to the initial configuration, the solid fails to restore to the initial structure. The quantifiers for such structural changes can be the shape of the body (at a macroscopic level of observation) or a rearrangement of defects (at a microscopic level of observation). Unlike elasticity, plasticity is fundamentally a microscopic phenomenon. An elastic process brings about no permanent changes in the structure of the solid, thereby allowing the body to deform without any change in its microstructure. On the other hand, a plastic process necessarily involves a change in the microstructure of the body. To construct a continuum theory of plasticity would therefore require identifying the appropriate microstructural rearrangements and introducing suitable parameters for their representation. Before discussing the general theory, it will be helpful to understand the phenomenon of plasticity through a

simple one dimensional example.

## 1.1 Plasticity: the phenomenon

To illustrate the phenomenon of plasticity we consider a simple example of stretching a metal wire (with cylindrical cross-section) under an isothermal environment. A representative element of the wire is selected and the following two quantities are measured: the force per unit cross-sectional area (stress) and the change in length of the element with respect to some fixed reference state (strain). Two typical stress-strain plots thus obtained are shown in Figure 1.1.

Below a certain critical value of stress and strain, the element under observation returns to its original state of stress and strain upon removal of the external mechanism for stretching. The collection of all such stress/strain values forms the *elastic range* associated with the material. The deformation remains elastic as long as the stress/strain values are restricted to the elastic range. For values beyond the elastic range, the element will undergo permanent structural changes. The boundary of the elastic range signifies the onset of plastic deformation and therefore can be appropriately termed as the *yield limit* for the transition from an elastic to a plastic deformation process. It should however be noted that for most materials an accurate measurement of the yield limit is difficult because of the gradual nature of the transition from elastic to plastic behavior. It then becomes a matter of convention to choose an appropriate yield limit for such materials. Based on the nature of the yield limit, we distinguish between two models of plastic flow. The first model is known as perfect plasticity (or the ideal plastic flow), wherein the yield limit for

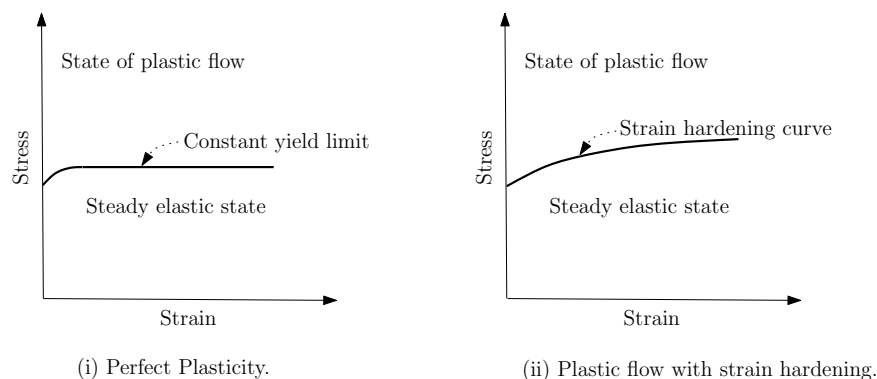


Figure 1.1: Simple stress–strain curves. (After Bridgman [22]).

stress is assumed to remain constant (Figure 1.1(i)). The second model, however, allows the yield stress to vary with the structural changes in the body (Figure 1.1(ii)). Before we go on to discuss these two models, note from Figure 1.1 that for a zero strain, the stress does not necessarily vanish. This can be attributed to the presence of microstructure in the form of defects in the unstrained state, which induces internal stresses so as to maintain an equilibrium configuration of defects in the element.

Let us first assume perfectly plastic behavior for the wire with a stress-strain curve of the form shown in Figure 1.1(i). Stretching the wire beyond the unstrained state using a tensile loading, the deformation process remains elastic until the stress in the element reaches the constant critical value (corresponding to the horizontal line in Figure 1.1(i)). The element (of the wire) under consideration will deform plastically as long as its stress state is maintained at the critical level, and will keep doing so till the onset of fracture (which can be understood as the catastrophic separation of the body into distinct parts [22]). If the wire is unloaded from the plastic state, it does so elastically. On loading the wire again, it will start to flow plastically on reaching the constant yield limit for stress.

The rate of plastic flow under constant yield stress depends on the load imposed at the boundary of the wire, as well as other physical properties of the wire. If, however, we try to load the wire such as to raise the stress in the element above the critical value, the element responds by an indefinite yielding. Such a plastic flow can no more be controlled via the force applied at the end of the wire, but is now dependent on the velocity with which the wire is stretched. This behavior is analogous to the free mobility of an ideal liquid.

In our actual experience, however, we find that we can indeed control the plastic flow via forces which bring the stress state to much higher levels than the initial yield stress. Moreover, most importantly in metals, we observe the phenomenon of hardening, where the solid tends to yield at higher and higher values of stress as a result of the change in its structure. Metals can be treated (e.g. cold worked) to bring desired structural changes, and can consequently be hardened (or softened) according to their industrial use. For example, the yield stress for pure aluminium and pure copper crystals can be increased a hundred fold by cold working [38]. The applicability of perfect plasticity is therefore limited to situations where strain hardening is absent. Such is indeed the case in experiments involving very high shear strains with high hydrostatic pressure (Chapter 16 in [22]) or when the deformations are very small [145].

This motivates us to consider the second model of plastic flow (Figure 1.1(ii)), where the yield limit for stress is no more constant, but is an increasing function of strain. Assume that we can impose any combination of stress and strain on the wire element. The response can then be divided into two parts of the stress–strain plane: a region of elastic states, and a region of plastic states, as shown in Figure 1.1(ii). A point in the elastic region



represents a steady elastic state and any deformation process from one point to another in the elastic region is an elastic process. A point in the plastic region, on the other hand, is unsteady and yields with a finite rate until it reaches a state at the boundary of plastic and elastic regions. This boundary is referred to as the strain hardening curve. To elaborate, let the wire be loaded beyond the zero strain state. At this point, the stress in the element might not be zero because of the internal stresses resulting from the microstructure. As the wire is loaded in tension, the stress and the strain values are measured (at the element) and are plotted as a curve in a stress-strain plane. The measurements are taken only after a steady value of stress/strain is reached. A typical curve thus obtained is shown in Figure 1.1(ii). For small increments of stress and strain, the response is elastic. Beyond a certain critical load, the wire starts to deform plastically. As the load is increased, the stress/strain state in the element might correspond to a point in the plastic region of the stress-strain plane. For a fixed load, the element will start to flow plastically for a finite time (unlike perfect plasticity) until it reaches the strain hardening curve. The rate of plastic flow will be, in general, a function of the state variables and the history of the state variables for the element. The magnitude of the rate will vary according to the distance of the state from the hardening curve. It will be slower near the hardening curve, but can become catastrophic when the initial imposed state is far from the hardening curve [22]. Once the element reaches a steady state on the hardening curve, we can unload the wire to bring the state of the element to the elastic region. On loading again, the element will now begin to yield at the state from which it was unloaded, where the stress value is higher than the stress at which yield first occurred. If the load is increased slowly from a state on the hardening

curve, the evolving states remain on the curve and we call this a rate-independent response of plastic flow. If however, the load is increased rapidly (or even moderately), the state might reach the plastic region, where the evolution of plastic flow is significantly different than that of the rate-independent flow. We call this response, the rate-dependent plastic flow. Therefore, during the plastic flow, the state remains on the yield surface (i.e. the strain hardening curve) for rate-independent plasticity, but can go beyond the yield surface into the plastic region for rate-dependent plasticity.

For a quantitative understanding of hardening, it would be necessary first to specify the fundamental mechanisms underlying plastic flow. As early as 1934, in their independent studies on plastic flow in metals, Orowan [136], Polanyi [144], and Taylor [162] conjectured dislocations to be the carriers of plastic flow. Since then, owing to much advancement in the experimental techniques of microscopy, it has become possible to observe dislocations and thereupon verify this conjecture [38, 3, 4]. A dislocation can be defined as a line defect of geometric nature, such that the integral of the gradient of displacement field along any closed curve around the defect line is non-zero. Along the dislocation line, the atomic structure deviates considerably from an otherwise perfect (i.e. without defect) solid. In ordered solids, for example crystals, the presence of dislocations disrupts the periodic nature of the lattice. The discovery of dislocations was initiated by the observation that metals start to deform plastically at much lower loads than they would for a perfect lattice structure. The stress required to move a dislocation is less than that required to move a row of atoms in a perfect lattice. Moreover, dislocations occur naturally in most crystals and only under special circumstances (e.g. high temperature) a crystal free of dislocations can be obtained.

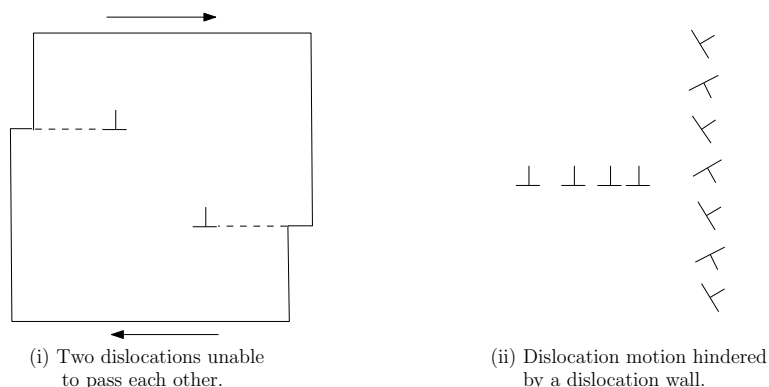


Figure 1.2: Mechanisms of hardening. (Figure (i) after Cottrell [38]).

The properties of a single dislocation in an elastic medium are well established and so are its interactions with other defects. The importance of dislocations have made them an active area of research in condense matter physics and many excellent expositions are available on the subject, see for e.g. Cottrell [38], Nabarro [122], Lardner [99], Teodosiu [164], Hirth & Lothe [76], and Weertman & Weertman [174].

It is then natural to expect that hardening is controlled by nucleation and mobility of dislocations, wherein the central role is played by the obstacles to the dislocations carrying plastic flow. Moving dislocations can face obstacles in the form of point defects (precipitates, vacancies), line defects (other dislocations, Figure 1.2(i)), and surfaces (grain boundaries, Figure 1.2(ii), phase boundaries, rigid walls) [118, 38, 123, 4]. The hinderance is usually caused by the stress fields associated with obstacles which interact with the stress field of moving dislocations such that the net stress is in equilibrium. In such situations, additional stresses would then be needed to resume the motion of dislocations. Hardening depends on the group behavior of the microstructure and is therefore highly non-local in its character. On the other hand, the yield strength is further modified as more dislocations are nucleated.

Typical nucleation sites include sharp corners, crack tips, grain boundaries, and even the dislocation itself, which can nucleate more dislocations by acting as a Frank–Read source [38, 4].

## 1.2 Plasticity as a thermodynamically irreversible process

Plasticity, by virtue of inducing permanent structural changes, is a thermodynamically irreversible process. The methods of irreversible thermodynamics should therefore provide the basic framework for formulating a rational theory of plastic flow. In this section, we will motivate the fundamental ideas from thermodynamics, which are used in our theory of plasticity.

Divide the body into small material elements (a discussion on the size of these elements is given below), each of which is characterized by a collection of variables representing the thermodynamic state. In a continuum theory, every material element corresponds to a material point in the body. A material element is said to be in *equilibrium* if it forever remains in the same thermodynamic state under no external influence. A material element undergoes an *irreversible process* if the effects of the process cannot be reversed without bringing finite changes in the environment of the element. A complete description of the body, on the other hand, depends not only on the determination of states for each material element, but also on the interactions among the elements. Therefore, equilibrium of material elements (local equilibrium) does not necessarily imply equilibrium of the body (global equilibrium). Following theories of classical irreversible thermodynamics (see for e.g., Prigogine [146] and de Groot & Mazur [64]), we assume that the body always remains in local

equilibrium but not necessarily in global equilibrium. The size of material elements, should thus be such that it contains enough molecules for microscopic fluctuations to be negligible. It however, should be sufficiently small so as to capture the pertinent microstructural features of the body. With the assumption of local equilibrium, we can posit the existence of thermodynamic state variables such as temperature and entropy for each material element. In an out-of-equilibrium situation, it is not always possible to give a meaningful interpretation to these quantities [57, 33].

To begin with, a choice of state variables needs to be established. Next, the two laws of thermodynamics should be written in an appropriate form. As stated above, the behavior of the body depends not only on the state of individual material elements but also on the interaction of the body with the environment and the interaction among material elements. Therefore, the laws of thermodynamics should be written in an integral form for arbitrary parts of the body and subsequently localized to obtain local relations at various material elements. The first law of thermodynamics is a statement about balance of energy, while the second law of thermodynamics imposes the net internal entropy generation (dissipation) to be non-negative [146].

Bridgman [20] highlighted, with much correctness, that during plastic flow, the body is “completely surrounded by irreversibility”. However, in classical thermodynamics the laws are written for reversible processes and the concept of entropy is defined only as a difference between a final and an initial state which can be connected by some reversible process [142]. We avoid these problems by formulating the thermodynamic theory following Prigogine [146], as outlined above. Of course, for situations where microstructural fluctua-

tions might play an important role (for e.g. nucleation) and can not be neglected, we would have to either expand the space of state variables or to employ methods of statistical mechanics (much work has been done recently to study the dynamics of dislocations using the concepts of statistical mechanics, see for example [72, 123]). Our theory should therefore aim at resolving the microstructure only to the extent till we can support the hypothesis of local equilibrium.

The choice of state variables is of central importance to the development of the theory. The variables which qualify for describing the thermodynamic state should be observable, but not necessarily controllable. Observability of the variables is essential for any experimental verification of the premises and the results of the theory. A variable is controllable if there exists an external mechanism to independently control its value. For example, we can control the stretch of a wire by applying a suitable force. There are, on the other hand, variables which can not be controlled without affecting other variables. An example is furnished by the position of a single dislocation line in a solid, which can not be varied without affecting either the local strain field or the temperature field. Moreover, there does not exist a control mechanism which can be employed to vary the position of the dislocation line.

Finally, it is important to note that in most cases, the second law of thermodynamics proves to be insufficient for the determination of the evolution law for dissipative variables. It then becomes necessary to introduce additional postulates, such as principle of maximum entropy, which are then used to determine the evolution laws. The validity of such additional postulates should be experimentally verifiable, at least for the class of

materials for which they are used.

### 1.3 Continuum theories of plasticity

Historically, it was the interest in ascertaining the strength of materials, which led to the development of plasticity theory. The first known scientific studies, which date back to as early as the beginning of the nineteenth century [75], were to obtain the criteria for plastic yielding in soils and metals. Due to the microstructural nature of plastic deformation, a mathematical theory of plasticity has always depended on the state of experimental progress to observe (and measure) the phenomenon of plastic flow.

By the mid-twentieth century, an experimentally substantiated theory for rate-independent incompressible plastic flow in isotropic metals at ordinary temperatures was established. The main components of this theory were a yield criteria and a relation between stress and rate of plastic strain. One of the most successful yield criteria was proposed by von Mises, according to which the yield begins when a certain quadratic function of stress reaches a critical constant value. Extension of the von Mises criteria for anisotropic solids was first considered by Hill [75], and has been recently studied by Cazacu & Barlat [28]. To include the hardening effects, the criterion was generalized in the works of Taylor & Quinney, Schmidt, and Odquist [75], by replacing the constant critical value with a function of some hardening parameter. The hardening parameters were chosen to provide a suitable measure of the strain history and were usually represented by quantities like plastic work and plastic distortion [75]. On the other hand, Saint-Venant, Lévy, Prandtl, and Reuss [75, 82] proposed plastic flow rules which expressed the proportionality of deviatoric stress

and deviatoric rate of plastic strain. The plastic flow rule combined with the yield criteria, the equilibrium condition for stress, and the boundary conditions, were sufficient to solve a boundary value problem of macroscopic plastic flow [75, 22, 145, 165, 82].

A rate-dependent generalization was provided independently by Sokolovsky and Malvern, and advanced by Perzyna [140, 141]. The rate-dependent theory was motivated by the observation of higher yield values for high loading rates, and was found to be more suitable in the dynamic studies of plasticity [27, 132]. As noted earlier, the rate-dependent plastic flow does not restrict the stress state to lie on the yield surface, but allows it to go beyond it into an unsteady plastic regime. The nature of flow rules for a rate-dependent response is therefore significantly different from rate-independent response, as they would now have to include appropriate time scales for the relaxation of plastic deformation.

The next few decades after the mid-twentieth century saw two important advancements to rigorously establish a mathematical theory of plasticity. The two developments, which remained mostly independent, were concerning the geometric and the thermodynamic nature of plastic flow. It was clear by this time that dislocations were the fundamental objects responsible for plasticity. Due to their high density, they were considered not as discrete objects but as continuously spread over the body. A geometric theory of the body with a continuous distribution of dislocations was first formulated by Kondo [88] and Bilby [14]. Subsequent advancements were made by Kröner [93], Noll [129], and Edelen [83]. In these theories, the dislocation distribution is characterized by an affine connection (torsion) and a metric associated with the body manifold. The physical nature of a distribution of dislocations can be understood from the following thought example: Consider the body



as given to the experimentalist and divide it into several small parts, so as to relax the stress in each sub-part of the body. It might be necessary to cut the parts infinitesimally small. If these parts do not fit together (without forming holes etc.), we say that the body is dislocated (or inhomogeneous, according to Noll [129]).

Parallel to these geometric developments, were attempts to formulate a thermodynamic theory of plasticity. On one hand, starting from the papers of Eckart [44] and Bridgman [20], it became increasingly evident that a general theory of plasticity had to rest on the fundamental laws of thermodynamics. The first such theories were presented by Kestin [84, 86] and Green & Naghdi [61, 124], both of which introduced plastic strain as the internal variable whose evolution contributes to the dissipation. And on the other hand, postulates of maximum dissipation were provided by Drucker [43] and Ilyushin [80], which not only established plastic flow rules for rate-independent materials but also provided restrictions on the nature of the yield surface. The postulate of maximum plastic dissipation is a stronger inequality than the second law of thermodynamics [112], which in itself is insufficient to establish a plastic flow rule.

The last two decades of the twentieth century (extending to the present) saw significant advances in computational and experimental techniques. As a result, it was no longer required to solve the complete problem analytically, nor it was needed to restrict the variables to the coarse scale of observations. Large scale computations could now be done where using the properties of single dislocations, dynamics of millions of interacting dislocations were simulated [24]. On the other hand, several new micro-scale experiments emphasized the emergence of size effects and novel mechanisms for strain hardening [4].

It thus became imperative for a continuum theory of plasticity to expand its horizon so as to be able to predict a wide class of phenomena, although maintaining computational feasibility and experimental verifiability. New attempts were made to pose the boundary value problem for plastic flow, either by prescribing independent laws for the evolution of dislocation density [1] or by enriching the basic continuum theory to include gradient effects [52, 68].

The aim of this thesis is two fold. First, we construct a framework for a general theory of anisotropic thermoplasticity, with an aim to encompass previously established models and several seemingly independent lines of research. The theory is based on the two laws of thermodynamics and basic invariance requirements. Invariance is imposed under arbitrary changes in the reference configuration, frame indifference, and material symmetry. The interplay between constitutive assumptions and the kinematics is, in particular, emphasized. The classical models of plastic flow are deduced under additional assumptions and a few explicit results are obtained for materials with cubic symmetry. Second, we study interfaces in a plastically deforming solid. The interfaces are assumed to be in the form of waves (shock waves and acceleration waves), grain boundaries, and phase boundaries. The concept of surface dislocations is rigorously established and the governing equations for the dynamics of shock waves and acceleration waves are obtained. In addition, simple examples demonstrating the behavior of these plastic waves are considered. Finally a theory, where the interface itself contributes energetically, is constructed. The resulting formulation provides us with a basis to study the coupling between grain boundary migration and accompanying plastic flow.

The future too looks increasingly vibrant for the development of plastic flow theories. The phenomenon offers a physical setup to study the dynamics of matter across several time and length scales. The concepts of condensed matter physics, non-linear thermodynamics, and continuum mechanics have to be combined to formulate a well-founded theory of plasticity with an aim to understand both the micro-scale and the macro-scale behavior of solids, with deformation processes occurring for a wide range of time durations (from instantaneous pattern formation to creep).

## 1.4 Overview of the thesis

In Chapter 2, we provide a brief but rigorous introduction to continuum mechanics and thermodynamics with an aim to make this thesis self contained. The chapter begins by introducing fundamental concepts of the body, its deformation, and its motion. Many relevant results from linear algebra and mathematical analysis are stated and proved. For the study of interfaces, we introduce the notion of a singular surface in the body. Singular surfaces are two dimensional surfaces in the three dimensional body, across which kinematical fields (like deformation, motion, and possibly their gradients) suffer jump discontinuities. Such discontinuities are used to model waves, grain boundaries, and phase boundaries. In the second part of Chapter 2, we formulate the basic laws of continuum thermodynamics. As a necessary preliminary, we discuss various integral theorems, which are used to extract localized equations from their integral counterparts. The balance of mass, momentum, and energy are stated first in a global form for arbitrary parts of the body. From these global equations, local relations of the balance laws are obtained, to be satisfied by material points

away from the singular surface and on the singular surface. The chapter ends with the second law of thermodynamics, which postulates the non-negativity of the internal entropy for arbitrary parts of the body. Local inequalities are derived to be satisfied by the dissipation at material points away from and on the singular surface.

In Chapter 3, we lay down the framework for a thermodynamic theory of anisotropic plastic flow with finite deformations. The permanent changes are assumed to be brought via motion of dislocations and singular surfaces. We begin by examining the basis of the idea of a local stress-free state, and an associated manifold of intermediate configurations. This is grounded in the notion of an equilibrium unloading process together with appropriate constitutive hypotheses on the elastic response. Next, the constituent elastic and plastic deformations are discussed. Stokes' theorem is used to describe the concepts of incompatibility and the associated dislocation density. The notion of geometrically necessary and statistically stored dislocation densities is also clarified. One of the central results in this chapter is to obtain the restrictions on a constitutive function to be independent of compatible changes in the reference configuration. The basis for such an invariance is the fact that our choice of a reference configuration is arbitrary and therefore should not have any influence on the material response. The basic thermodynamic framework is then discussed, where the elasticity of the body is described and the dissipation associated with the plastic evolution is expressed in terms of Eshelby's tensor. Material symmetry restrictions on the elastic response and on constitutive equations for yield and plastic flow are subsequently discussed. Finally, we use various invariance requirements to obtain a general form of the flow rule and the yield criteria. The latitude afforded by the constitutive character

of the plastic deformation is used to dispose of a long-standing controversy surrounding plastic spin. The chapter concludes with detailed remarks on work hardening, size effects, symmetry groups, and Bauschinger effect.

The aim of Chapter 4 is to revisit the theory developed in Chapter 3 under assumptions on the nature of elastic strain. We start with a postulate of Ilyushin, according to which the plastic work is always non-negative for a process with coinciding initial and final deformation gradient fields. This postulate furnishes a sufficient condition for obtaining associated flow rules and a convex yield surface. Next, we assume the elastic strain to be infinitesimally small, but still allowing for finite rotations and finite plastic strain. After reducing our general theory in the light of this assumption, we discuss, in detail, the nature of associated flow rules in the absence and presence of hardening. Finally, we concern ourselves with elastically rigid and perfectly plastic solids. For elastically rigid solids, the elastic strain is assumed to vanish completely, thereby reducing the elastic distortion to a rotation. The stress is indeterminate in such a situation (since there is no strain energy), but it can be understood as the Lagrange multiplier associated with the constraint of imposing the elastic distortion to be a rotation. The assumption of perfectly plastic behavior requires absence of any hardening in the model. Therefore, we consider the flow rules and yield criterion to be independent of dislocation density. The theory of elastically rigid perfectly plastic bodies is fundamentally different from what we have modeled so far, as the notion of stress is no longer constitutive and derived from an energy, but is rather of the nature of a Lagrange multiplier.

Chapter 5 is divided into two parts. The first part deals with the general theory

of surface dislocation density and the second part is concerned with the theory of adiabatic plastic waves. The concept of surface dislocation density arises from a discontinuous plastic distortion or a discontinuous elastic distortion, both of which lack the usual rank one jump condition in the presence of surface dislocations. We obtain compatibility conditions to be satisfied at a surface dislocation node, which is the line at which several dislocated surfaces intersect. A measure of surface dislocation density, which is invariant with respect to compatible changes in the reference configuration, is obtained. Finally, the jump in bulk dislocation density is related to the surface dislocation density. For a moving surface, the jump is given completely in terms of the jump in plastic distortion rate and the surface dislocation density. In particular, a statement of the conservation of dislocation density at the surface, according to which, the normal component of the jump in bulk dislocation density is equal to the surface divergence of the surface dislocation density.

In the second part of Chapter 5, we develop a theory of shock waves and accelerations waves in a plastically deforming medium. A wave is understood to be a moving singular surface, across which fields and their derivatives might suffer jump discontinuities. Shock waves are singular surfaces across which the thermodynamic state variables are discontinuous and acceleration waves are singular surfaces across which the thermodynamic state variables are continuous but their first derivatives are discontinuous. We begin by obtaining some general results for elastic shock waves. In particular we show that the jump in entropy is of the third order in the jump in deformation gradient, and the change in entropy is of the same sign as of the change in shock speed. Next, we investigate on how these results of elastic shocks modify due to the presence of plastic flow at the shock surface.

We find that the jump in entropy, for a fixed plastic flow, is of the first order in the jump in deformation gradient. As a simple example of plastic shock waves, we consider the shock as a dislocation wall, i.e. a surface with continuous distribution of dislocations. We obtain simple equations, which for given material parameters can be used to determine the dislocation density distribution at the shock as well as the shock speed. Results are obtained for both isotropic and cubic material symmetry. We then move on to discuss adiabatic acceleration waves in elastic–plastic solids. The form of governing equations for acceleration waves make them much more analytically tractable than shock waves. A general theory of elastic–plastic acceleration waves is formulated and the role of dislocation distribution near the wave is emphasized. Some classical results on the form of elastic acoustic tensor for isotropic and cubic material symmetry are derived. As examples, plastic acceleration waves with rate–independent behavior are discussed with and without hardening.

The final chapter is primarily concerned with two results. The first is to obtain the restrictions on constitutive functions, defined on the interface, on using their invariance under compatible changes in the reference configuration. Such an invariance is to be naturally expected of the constitutive functions, which should not depend on our choice of a reference configuration. As an interesting conclusion, we show that constitutive functions can depend on plastic distortion only through the true surface dislocation density. The second result is to reformulate the thermodynamics of plastic flow, but with the addition of interfacial stresses and interfacial energy, thus endowing an independent constitutive structure to the interface. The resulting theory provides, for example, the basic framework for studying the problem of accompanying plastic deformation during grain/phase boundary migration.

## Chapter 2

# Continuum Mechanics<sup>1</sup>

The purpose of this chapter is to present a review of pertinent concepts from continuum mechanics which will be used in rest of the thesis. This also serves our aim to make this work self contained. The chapter is divided into two parts. The first part deals with fundamental notions associated with the kinematics of a continuous body. In particular, singular surfaces, across which kinematical variables (such as velocity and deformation gradient) may be discontinuous, are discussed in sufficient detail. The second part of this chapter introduces universal balance laws which govern the mechanics of continuous bodies. Local statements of the balance laws concerning mass, momentum and energy are obtained at points away from the singular surface and also at points on the singular surface. In Remark 2.2.4 we use classical invariance properties to derive the balance of mass and momentum from the balance of energy. The chapter concludes with the section on the second law of thermodynamics and its consequences for irreversible processes in a continuous

---

<sup>1</sup>A modified version of this chapter has been submitted for publication in a forthcoming Encyclopedia [65].



media.

For further reading, the interested reader is referred to many excellent expositions available on the subject. A few, which guided most of the content of this chapter, are by Truesdell [171, 170], Noll [131], Chadwick [32], Gurtin [67] and Šilhavý [156].

The following notation is adopted in which  $\mathcal{V}$  is the translation (vector) space of a real three-dimensional Euclidean point space  $\mathcal{E}$ :

*Lin*: the linear space of linear transformations (tensors) from  $\mathcal{V}$  to  $\mathcal{V}$ .

*InvLin*: the group of invertible tensors.

*Sym* =  $\{\mathbf{A} \in Lin : \mathbf{A} = \mathbf{A}^T\}$ , where superscript  $T$  denotes the transpose: linear space of symmetric tensors; also, the linear operation of symmetrization on *Lin*.

*Sym*<sup>+</sup> =  $\{\mathbf{A} \in Sym : \mathbf{u} \cdot \mathbf{A}\mathbf{u} > 0\}$  for  $\mathbf{u} \neq \mathbf{0}, \mathbf{u} \in \mathcal{V}$ : the positive-definite tensors.

*Skw* =  $\{\mathbf{A} \in Lin : \mathbf{A}^T = -\mathbf{A}\}$ : the linear space of skew tensors; also, the linear operation of skew-symmetrization on *Lin*.

*Orth* =  $\{\mathbf{A} \in InvLin : \mathbf{A}^T = \mathbf{A}^{-1}\}$ , where  $\mathbf{A}^{-1}$  is the inverse of  $\mathbf{A}$ : the group of orthogonal tensors.

*Orth*<sup>+</sup> =  $\{\mathbf{A} \in Orth : J_A = 1\}$ : the group of rotations.

Here and in the following chapters, both indicial notation as well as bold notation is used to represent vector and tensor fields. The components in the indicial notation are written with respect to the Cartesian coordinate system. Indices denoted with roman alphabets vary from one to three but those denoted with Greek alphabets vary from one to two. Einstein's summation convention is assumed unless an exception is explicitly stated. Let  $e_{ijk}$  be the three dimensional permutation symbol, i.e.  $e_{ijk} = 1$  or  $e_{ijk} = -1$  when

$(i, j, k)$  is an even or odd permutation of  $(1, 2, 3)$ , respectively, and  $e_{ijk} = 0$  otherwise.

The determinant and cofactor of  $\mathbf{A}$  are denoted by  $J_A$  and  $\mathbf{A}^*$ , respectively, where  $\mathbf{A}^* = J_A \mathbf{A}^{-T}$  if  $\mathbf{A} \in \text{InvLin}$ . It follows easily that  $(\mathbf{AB})^* = \mathbf{A}^* \mathbf{B}^*$ . Further,  $\text{Lin}$  is equipped with the Euclidean inner product and norm defined by  $\mathbf{A} \cdot \mathbf{B} = \text{tr}(\mathbf{AB}^T)$  and  $|\mathbf{A}|^2 = \mathbf{A} \cdot \mathbf{A}$ , respectively, where  $\text{tr}(\cdot)$  is the trace operator. We make frequent use of relations like  $\mathbf{A} \cdot \mathbf{BC} = \mathbf{AC}^T \cdot \mathbf{B} = \mathbf{C}^T \cdot \mathbf{A}^T \mathbf{B}$  and  $\mathbf{AB} \cdot \mathbf{CD} = \mathbf{ABD}^T \cdot \mathbf{C}$ , etc., which follow easily from  $\text{tr} \mathbf{A} = \text{tr} \mathbf{A}^T$  and  $\text{tr}(\mathbf{AB}) = \text{tr}(\mathbf{BA})$ . It is well known that  $\text{Lin} = \text{Sym} \oplus \text{Skw}$ , the direct sum of  $\text{Sym}$  and  $\text{Skw}$ . The tensor product  $\mathbf{a} \otimes \mathbf{b}$  of vectors  $\{\mathbf{a}, \mathbf{b}\} \in \mathcal{V}$  is defined by  $(\mathbf{a} \otimes \mathbf{b})\mathbf{v} = (\mathbf{b} \cdot \mathbf{v})\mathbf{a}$  for all  $\mathbf{v}$  in  $\mathcal{V}$ , where  $\mathbf{b} \cdot \mathbf{v}$  is the standard inner product of vectors.

A fourth order tensor is a linear transformation  $\mathcal{A} : \text{Lin} \rightarrow \text{Lin}$ . Its operation on a second order tensor is represented by  $\mathbf{A} = \mathcal{A}[\mathbf{B}]$  for  $\{\mathbf{A}, \mathbf{B}\} \in \text{Lin}$ . In terms of indices, this is written as  $A_{ij} = \mathcal{A}_{ijkl} B_{kl}$ . A fourth order unit tensor  $\mathbb{I}$  is defined as  $\mathbb{I}[\mathbf{A}] = \mathbf{A}$  for every  $\mathbf{A} \in \text{Lin}$ . In components,  $\mathbb{I}_{ijkl} = \delta_{ik} \delta_{jl}$ . A tensor product  $\mathbf{A} \otimes \mathbf{B}$  of two second order tensors is a fourth order tensor defined by  $(\mathbf{A} \otimes \mathbf{B})[\mathbf{C}] = (\mathbf{C} \cdot \mathbf{B})\mathbf{A}$ , for  $\mathbf{C} \in \text{Lin}$ . The major transpose of a fourth order tensor  $\mathcal{A}$  is a fourth order tensor  $\mathcal{A}^\mathbb{T}$  defined by  $\mathcal{A}^\mathbb{T}[\mathbf{B}] \cdot \mathbf{A} = \mathbf{B} \cdot \mathcal{A}[\mathbf{A}]$ . Moreover,  $\mathcal{A}$  has a major symmetry if  $\mathcal{A}^\mathbb{T} = \mathcal{A}$ , or in indices  $\mathcal{A}_{ijkl} = \mathcal{A}_{klij}$ . It has a minor symmetry of the first kind, if it is symmetric with respect to first two indices, i.e. if  $(\mathcal{A}[\mathbf{B}])^T = \mathcal{A}[\mathbf{B}]$ , for  $\mathbf{B} \in \text{Lin}$ . The tensor  $\mathcal{A}$  has a minor symmetry of a second kind, if it is symmetric with respect to last two indices, i.e. if  $\mathcal{A}[\mathbf{B}^T] = \mathcal{A}[\mathbf{B}]$ . A fourth order tensor  $\mathcal{A}$  is invertible if there exists another fourth order tensor  $\mathcal{B}$  such that  $\mathcal{AB} = \mathbb{I}$ , or in components  $\mathcal{A}_{ijkl} \mathcal{B}_{klmn} = \mathbb{I}_{ijmn}$ . The tensor  $\mathcal{B}$  is then called the inverse of  $\mathcal{A}$  and is denoted by  $\mathcal{A}^{-1}$ .

## 2.1 Kinematics

In this section we begin by introducing the notion of a body, its configurations and its motion. Derivatives of scalar, vector and tensor fields are then defined, followed by a discussion on the deformation gradient and its various properties. Finally, we introduce the kinematics associated with a two dimensional surface. Such a surface is called singular if any of the kinematic variable (or its higher order derivative) is discontinuous across it. Compatibility conditions, which relate the values of the discontinuous kinematic variable across the surface, are also obtained.

### 2.1.1 Body, configurations and motion

The geometrical structure of a physical body is independent of a frame of reference, and therefore the *body* (in continuum mechanics) is usually taken to be a three dimensional differential manifold. We denote such a manifold by  $\mathfrak{B}$  and call its elements material points. At every material point  $X \in \mathfrak{B}$  we have an associated tangent space  $\mathcal{T}_X$  which is a three dimensional vector space representing a neighborhood of  $X$ . On the other hand, the body is observed and tested in a (three dimensional) Euclidean frame of reference  $\mathcal{E}$ , which requires us to endow the body  $\mathfrak{B}$  with a class  $\mathcal{C}$  of bijective mappings,  $\chi : \mathfrak{B} \rightarrow \mathcal{E}_\chi$  (the subscript  $\chi$  is used to indicate the mapping employed). We call these mappings the *configurations* of the body  $\mathfrak{B}$ . The spatial position  $\chi(X) \in \mathcal{E}_\chi$  denotes the *place* which a material point  $X \in \mathfrak{B}$  occupies in  $\mathcal{E}_\chi$ . The translation space of  $\mathcal{E}_\chi$  is a three dimensional inner product space, and is denoted by  $\mathcal{V}_\chi$ .

We introduce a fixed *reference configuration*, relative to which the notions of dis-

placement and strain can be defined. Let  $\boldsymbol{\kappa} \in \mathbf{C}$  be a reference configuration. The configuration  $\boldsymbol{\kappa}$  need not be a configuration occupied by  $\mathfrak{B}$  at any time and therefore  $\boldsymbol{\kappa}$  can be arbitrary as long as it belongs to  $\mathbf{C}$ .

The *motion* of a body  $\mathfrak{B}$  is defined as a one-parameter family of configurations,  $\boldsymbol{\chi}_t : \mathfrak{B} \times \mathbb{R} \rightarrow \mathcal{E}_\chi$ . Such a motion assigns a place  $\mathbf{x} \in \mathcal{E}_\chi$  to the material point  $X \in \mathfrak{B}$  at time  $t$ . We write this as

$$\mathbf{x} = \boldsymbol{\chi}_t(X) \equiv \boldsymbol{\chi}(X, t). \quad (2.1)$$

The reference configuration  $\boldsymbol{\kappa}$  assigns a place  $\mathbf{X} \in \mathcal{E}_\kappa$  to  $X$ , so we can express  $\mathbf{x}$  as a function of  $\mathbf{X}$ ,

$$\mathbf{x} = \boldsymbol{\chi}(\boldsymbol{\kappa}^{-1}(\mathbf{X}), t) \equiv \boldsymbol{\chi}_\kappa(\mathbf{X}, t), \quad (2.2)$$

where  $\boldsymbol{\chi}_\kappa : \mathcal{E}_\kappa \times \mathbb{R} \rightarrow \mathcal{E}_\chi$  denotes a mapping from the reference configuration to the configuration of the body at time  $t$ .

The *displacement*  $\mathbf{u} : \mathfrak{B} \times \mathbb{R} \rightarrow \mathcal{V}$  ( $\mathcal{V}$  can be identified with either  $\mathcal{V}_\chi$  or  $\mathcal{V}_\kappa$ ) of a material point  $X$  with respect to the reference configuration  $\boldsymbol{\kappa}$  at time  $t$  is defined as

$$\mathbf{u}(X, t) = \boldsymbol{\chi}(X, t) - \boldsymbol{\kappa}(X). \quad (2.3)$$

The particle *velocity*  $\mathbf{v} : \mathfrak{B} \times \mathbb{R} \rightarrow \mathcal{V}_\chi$  and the particle *acceleration*  $\mathbf{a} : \mathfrak{B} \times \mathbb{R} \rightarrow \mathcal{V}_\chi$  are defined as

$$\mathbf{v}(X, t) = \frac{\partial}{\partial t} \boldsymbol{\chi}(X, t) \quad (2.4)$$

and

$$\mathbf{a}(X, t) = \frac{\partial^2}{\partial t^2} \boldsymbol{\chi}(X, t), \quad (2.5)$$

respectively. Displacement, particle velocity and particle acceleration can all be alternatively expressed as functions on  $\boldsymbol{\kappa}(\mathfrak{B})$  by using the inverse  $\boldsymbol{\kappa}^{-1} : \mathcal{E}_\kappa \rightarrow \mathfrak{B}$ . Such functions

exist in a one-to-one relation with the functions expressed in the equations above. We write

$$\begin{aligned}\hat{\mathbf{u}}(\mathbf{X}, t) &\equiv \mathbf{u}(\boldsymbol{\kappa}^{-1}(\mathbf{X}), t) \\ \hat{\mathbf{v}}(\mathbf{X}, t) &\equiv \mathbf{v}(\boldsymbol{\kappa}^{-1}(\mathbf{X}), t) \\ \hat{\mathbf{a}}(\mathbf{X}, t) &\equiv \mathbf{a}(\boldsymbol{\kappa}^{-1}(\mathbf{X}), t).\end{aligned}\tag{2.6}$$

We can similarly write these functions as

$$\begin{aligned}\tilde{\mathbf{u}}(\mathbf{x}, t) &\equiv \mathbf{u}(\boldsymbol{\chi}_t^{-1}(\mathbf{x}), t) \\ \tilde{\mathbf{v}}(\mathbf{x}, t) &\equiv \mathbf{v}(\boldsymbol{\chi}_t^{-1}(\mathbf{x}), t) \\ \tilde{\mathbf{a}}(\mathbf{x}, t) &\equiv \mathbf{a}(\boldsymbol{\chi}_t^{-1}(\mathbf{x}), t).\end{aligned}\tag{2.7}$$

We define the *material time derivative* as the derivative of a function with respect to time for a fixed material point. For an arbitrary scalar function  $f : \mathfrak{B} \times \mathbb{R} \rightarrow \mathbb{R}$ , we denote its material time derivative as  $\dot{f}$ . Thus,

$$\dot{f} = \frac{\partial}{\partial t} f(\mathbf{X}, t) |_{\mathbf{X}}.\tag{2.8}$$

If  $f$  is instead given in terms of  $\mathbf{x}$ , i.e. if  $f = \tilde{f}(\boldsymbol{\chi}(\mathbf{X}, t), t)$ , we write

$$\dot{f} = \frac{\partial}{\partial t} \tilde{f}(\mathbf{x}, t) |_{\mathbf{x}} + (\text{grad } \tilde{f}) \cdot \mathbf{v},\tag{2.9}$$

where  $\frac{\partial}{\partial t} \tilde{f}(\mathbf{x}, t) |_{\mathbf{x}}$  is the *spatial time derivative* (at a fixed  $\mathbf{x}$ ) and  $\text{grad } \tilde{f}$  is the spatial gradient (gradient is defined below). Therefore, if the particle velocity is a function of spatial position  $\mathbf{x}$ , then the particle acceleration is  $\tilde{\mathbf{a}} = \frac{\partial}{\partial t} \tilde{\mathbf{v}}(\mathbf{x}, t) |_{\mathbf{x}} + \mathbf{L}\mathbf{v}$ , where  $\mathbf{L} = \text{grad } \tilde{\mathbf{v}}$  is the spatial velocity gradient.

### 2.1.2 Derivatives

By *fields* we mean scalar, vector and tensor valued functions defined on position ( $\mathbf{x}$  or  $\mathbf{X}$ ) and time ( $t$ ). In the following we are mainly concerned with the derivatives with respect to the position and therefore dependence of fields on time is suppressed.

A scalar-valued field  $\phi(\mathbf{X}) : \mathcal{E}_\kappa \rightarrow \mathbb{R}$  is differentiable at  $\mathbf{X}_0 \in \mathcal{U}(\mathbf{X}_0)$ , where  $\mathcal{U}(\mathbf{X}_0) \subset \mathcal{E}_\kappa$  is an open neighborhood of  $\mathbf{X}_0$ , if there exists a unique  $\mathbf{c} \in \mathcal{V}_\kappa$  such that

$$\phi(\mathbf{X}) = \phi(\mathbf{X}_0) + \mathbf{c}(\mathbf{X}_0) \cdot (\mathbf{X} - \mathbf{X}_0) + o(|\mathbf{X} - \mathbf{X}_0|), \quad (2.10)$$

where  $\frac{o(\epsilon)}{\epsilon} \rightarrow 0$  as  $\epsilon \rightarrow 0$ . We call  $\mathbf{c}(\mathbf{X}_0) = \nabla\phi|_{\mathbf{X}_0}$  (or  $\nabla\phi(\mathbf{X}_0)$ ) the *gradient* of  $\phi$  at  $\mathbf{X}_0$ . Consider a curve  $\mathbf{X}(u)$  in  $\mathcal{E}_\kappa$  parameterized by  $u \in \mathbb{R}$ . Let  $\psi(u) = \phi(\mathbf{X}(u))$  and  $\mathbf{X}_1 = \mathbf{X}(u_1)$ ,  $\mathbf{X}_0 = \mathbf{X}(u_0)$  for  $\{u_1, u_0\} \in \mathbb{R}$ . Then from (2.10),

$$\psi(u_1) - \psi(u_0) = \nabla\phi(\mathbf{X}_0) \cdot (\mathbf{X}_1 - \mathbf{X}_0) + o(|\mathbf{X}_1 - \mathbf{X}_0|). \quad (2.11)$$

Moreover  $\mathbf{X}_1 - \mathbf{X}_0 = \mathbf{X}'(u_0)(u_1 - u_0) + o(|u_1 - u_0|)$ , where  $\mathbf{X}'(u_0)$  is the derivative of  $\mathbf{X}$  with respect to  $u$  at  $u = u_0$ . Therefore,  $|\mathbf{X}_1 - \mathbf{X}_0| = O(|u_1 - u_0|)$  and consequently we can rewrite (2.11)

$$\frac{\psi(u_1) - \psi(u_0)}{u_1 - u_0} = \nabla\phi(\mathbf{X}_0) \cdot \mathbf{X}'(u_0) + \frac{o(|u_1 - u_0|)}{u_1 - u_0}. \quad (2.12)$$

For  $u_1 \rightarrow u_0$  we obtain *the chain rule*,  $\psi'(u_0) = \nabla\phi(\mathbf{X}(u_0)) \cdot \mathbf{X}'(u_0)$ , which can also be expressed as  $\frac{d\phi}{du} = \nabla\phi(\mathbf{X}) \cdot \frac{d\mathbf{X}}{du}$  or

$$d\phi(\mathbf{X}) = \nabla\phi(\mathbf{X}) \cdot d\mathbf{X}. \quad (2.13)$$

A vector-valued field  $\mathbf{v}(\mathbf{X}) : \mathcal{E}_\kappa \rightarrow \mathcal{V}$  is differentiable at  $\mathbf{X}_0 \in \mathcal{U}(\mathbf{X}_0)$  if there exists a unique tensor  $\mathbf{l} : \mathcal{V}_\kappa \rightarrow \mathcal{V}$  such that

$$\mathbf{v}(\mathbf{X}) = \mathbf{v}(\mathbf{X}_0) + \mathbf{l}(\mathbf{X}_0)(\mathbf{X} - \mathbf{X}_0) + \mathbf{r}, \quad (2.14)$$

where  $|\mathbf{r}| = o(|\mathbf{X} - \mathbf{X}_0|)$ . We call  $\mathbf{l}(\mathbf{X}_0) = \nabla \mathbf{v}|_{\mathbf{X}_0}$  (or  $\nabla \mathbf{v}(\mathbf{X}_0)$ ) the *gradient* of  $\mathbf{v}$  at  $\mathbf{X}_0$ . The chain rule in this case can be obtained following the procedure preceding (2.13):

$$d\mathbf{v}(\mathbf{X}) = (\nabla \mathbf{v})d\mathbf{X}. \quad (2.15)$$

The *divergence* of a vector field is a scalar defined by

$$\text{Div } \mathbf{v} = \text{tr}(\nabla \mathbf{v}). \quad (2.16)$$

The *curl* of a vector field is a vector defined by

$$(\text{Curl } \mathbf{v}) \cdot \mathbf{c} = \text{Div}(\mathbf{v} \times \mathbf{c}) \quad (2.17)$$

for any fixed  $\mathbf{c} \in \mathcal{V}$ .

Differentiability of a tensor-valued function is defined in a similar manner. In particular, for a tensor  $\mathbf{A}(\mathbf{X}) : \mathcal{E}_\kappa \rightarrow \text{Lin}$ , where  $\text{Lin}$  denotes the set of all linear maps from  $\mathcal{V}$  to  $\mathcal{V}$  (the set of all second order tensors), we write

$$d\mathbf{A}(\mathbf{X}) = (\nabla \mathbf{A})d\mathbf{X}. \quad (2.18)$$

The *divergence* of  $\mathbf{A}$  is the vector defined by

$$(\text{Div } \mathbf{A}) \cdot \mathbf{c} = \text{Div}(\mathbf{A}^T \mathbf{c}) \quad (2.19)$$

for any fixed  $\mathbf{c} \in \mathcal{V}$ . The superscript  $T$  denotes the transpose. The *curl* of  $\mathbf{A}$  is the tensor defined by

$$(\text{Curl } \mathbf{A})\mathbf{c} = \text{Curl}(\mathbf{A}^T \mathbf{c}) \quad (2.20)$$

for any fixed  $\mathbf{c} \in \mathcal{V}$ .

Finally, if the fields are expressed as functions of  $\mathbf{x}$  rather than  $\mathbf{X}$ , the various definitions above remain valid. In this case we denote the gradient, divergence and curl operators by  $\text{grad}$ ,  $\text{div}$  and  $\text{curl}$ , respectively.

### 2.1.3 Deformation gradient

If the mapping  $\chi_\kappa(\mathbf{X}, t)$  is differentiable with respect to  $\mathbf{X}$ , then we define the deformation gradient by

$$\mathbf{F} = \nabla \chi_\kappa. \quad (2.21)$$

Since  $\chi_\kappa(\mathbf{X}, t)$  is invertible for each  $\mathbf{X} \in \mathcal{E}_\kappa$ , the deformation gradient  $\mathbf{F}$  belongs to a family of invertible linear maps from the translation space of  $\mathcal{E}_\kappa$  to the translation space of  $\mathcal{E}_\chi$ , i.e.  $\mathbf{F} \in \text{InvLin}$ . This follows from the inverse function theorem ([152], page 221). For  $\{\mathbf{X}, \mathbf{Y}\} \in \mathcal{E}_\kappa$  equation (2.14) becomes

$$\chi_\kappa(\mathbf{Y}, t) = \chi_\kappa(\mathbf{X}, t) + \mathbf{F}(\mathbf{X}, t)(\mathbf{Y} - \mathbf{X}) + \mathbf{r} \quad (2.22)$$

and the chain rule (2.15) takes the form (for fixed  $t$ )

$$d\mathbf{x} = \mathbf{F}d\mathbf{X}, \quad (2.23)$$

where the differentials  $d\mathbf{X}$  and  $d\mathbf{x}$  belong to the translation spaces  $\mathcal{V}_\kappa$  at  $\mathbf{X}$  and  $\mathcal{V}_\chi$  at  $\mathbf{x}$ , respectively.

We now obtain relationships for transforming infinitesimal area and volume elements. Let  $d\mathbf{X}_1 \in \mathcal{V}_\kappa$  and  $d\mathbf{X}_2 \in \mathcal{V}_\kappa$  be two linearly independent infinitesimal line elements at  $\mathbf{X}$ . An infinitesimal area element can be constructed using these line elements, with area given by  $da_\kappa = |d\mathbf{X}_1 \times d\mathbf{X}_2|$  and the associated direction given by the unit normal  $\mathbf{n}_\kappa$  such



that  $\mathbf{n}_\kappa da_\kappa = d\mathbf{X}_1 \times d\mathbf{X}_2$ . In the configuration  $\chi_t$  the line elements  $d\mathbf{X}_1$  and  $d\mathbf{X}_2$  are transformed into line elements  $d\mathbf{x}_1 \in \mathcal{V}_\chi$  and  $d\mathbf{x}_2 \in \mathcal{V}_\chi$ , respectively at  $\mathbf{x} = \chi_\kappa(\mathbf{X}, t)$ . We obtain, using relation (2.23),  $d\mathbf{x}_1 = \mathbf{F}d\mathbf{X}_1$  and  $d\mathbf{x}_2 = \mathbf{F}d\mathbf{X}_2$ . The area element constructed using these line elements has area  $da = |d\mathbf{x}_1 \times d\mathbf{x}_2|$  with unit normal  $\mathbf{n}$  given by  $\mathbf{n}da = d\mathbf{x}_1 \times d\mathbf{x}_2$ . Therefore,

$$\begin{aligned} \mathbf{n}da &= \mathbf{F}d\mathbf{X}_1 \times \mathbf{F}d\mathbf{X}_2 \\ &= \mathbf{F}^*(d\mathbf{X}_1 \times d\mathbf{X}_2) \\ &= \mathbf{F}^*\mathbf{n}_\kappa da_\kappa. \end{aligned} \tag{2.24}$$

As  $\mathbf{F} \in \text{InvLin}$ , we have

$$\mathbf{F}^* = J_F \mathbf{F}^{-T}. \tag{2.25}$$

Consider a third line element  $d\mathbf{X}_3 \in \mathcal{V}_\kappa$  at  $\mathbf{X}$  such that the set  $\{d\mathbf{X}_1, d\mathbf{X}_2, d\mathbf{X}_3\}$  is linearly independent and positively oriented. The infinitesimal volume element associated with the reference configuration is then given by  $dv_\kappa = d\mathbf{X}_1 \cdot d\mathbf{X}_2 \times d\mathbf{X}_3$ . In configuration  $\chi_t$  the volume element at  $\mathbf{x} = \chi_\kappa(\mathbf{X}, t)$  is  $dv = d\mathbf{x}_1 \cdot d\mathbf{x}_2 \times d\mathbf{x}_3$  with  $d\mathbf{x}_3 = \mathbf{F}d\mathbf{X}_3$ . Therefore,

$$\begin{aligned} dv &= \mathbf{F}d\mathbf{X}_1 \cdot \mathbf{F}d\mathbf{X}_2 \times \mathbf{F}d\mathbf{X}_3 \\ &= \mathbf{F}d\mathbf{X}_1 \cdot \mathbf{F}^*(d\mathbf{X}_2 \times d\mathbf{X}_3) \\ &= J_F dv_\kappa \end{aligned} \tag{2.26}$$

and accordingly, if  $\kappa$  is a configuration that could be attained in the course of the motion of  $\mathfrak{B}$ , we require  $J_F > 0$  to ensure that a volume in  $\kappa$  corresponds to a volume in  $\chi$ .

**Material curves** Consider a curve  $C \subset \mathcal{E}_\kappa$  and parameterize it with a real number  $s \in \mathbb{R}$  such that  $C : \mathbb{R} \rightarrow \mathcal{E}_\kappa$ . We call  $C$  a *material curve*. Its placement in the configuration  $\chi$  is

denoted by  $c$  and we use  $s$  to parameterize it such that  $c : \mathbb{R} \rightarrow \mathcal{E}_\chi$ . Using the definition of the deformation gradient and assuming the mappings  $C$  and  $c$  to be differentiable, we write

$$\mathbf{x}'(s) = \mathbf{F}\mathbf{X}'(s). \quad (2.27)$$

If  $s$  is the arc-length on  $C$ , then the vector  $\mathbf{X}'(s)$  defines a unit tangent vector (denoted  $\mathbf{M}$ ) to the curve  $C$  at arc-length station  $s$ . Let  $\mathbf{x}'(s) = \mu\mathbf{m}$  with  $|\mathbf{m}| = 1$  and  $\mu = |\mathbf{x}'(s)|$ .

Substituting these in (2.27), we obtain

$$\mu\mathbf{m} = \mathbf{F}\mathbf{M}. \quad (2.28)$$

Since  $\mathbf{F} \in \text{InvLin}$ ,  $\mathbf{F}\mathbf{M} \neq \mathbf{0}$  and therefore  $\mu > 0$ . We call  $\mu(s, t)$  the local stretch of  $C$ . It follows from (2.28) that

$$\mu^2 = |\mu\mathbf{m}|^2 = \mathbf{F}\mathbf{M} \cdot \mathbf{F}\mathbf{M} = \mathbf{M} \cdot \mathbf{C}\mathbf{M}, \quad (2.29)$$

where  $\mathbf{C} = \mathbf{F}^T\mathbf{F} : \mathcal{V}_\kappa \rightarrow \mathcal{V}_\kappa$  is the *Right Cauchy Green tensor*. The tensor  $\mathbf{C}$  is symmetric and positive definite, i.e.  $\mathbf{C} \in \text{Sym}^+$ . Indeed,  $\mathbf{C}^T = (\mathbf{F}^T\mathbf{F})^T = \mathbf{F}^T\mathbf{F} = \mathbf{C}$  and for arbitrary  $\mathbf{a} \in \mathcal{V}_\kappa$ ,  $\mathbf{a} \cdot \mathbf{C}\mathbf{a} = \mathbf{F}\mathbf{a} \cdot \mathbf{F}\mathbf{a} = |\mathbf{F}\mathbf{a}|^2 > 0$ , as  $J_F \neq 0$ . Similarly, if we rewrite (2.28) as  $\mu^{-1}\mathbf{M} = \mathbf{F}^{-1}\mathbf{m}$ , we can arrive at the (symmetric and positive definite) *Left Cauchy Green tensor*  $\mathbf{B} = \mathbf{F}\mathbf{F}^T : \mathcal{V}_\chi \rightarrow \mathcal{V}_\chi$  such that  $\mu^{-2} = \mathbf{m} \cdot \mathbf{B}^{-1}\mathbf{m}$ . We can use  $\mathbf{C}$  to calculate the deformed length of a material curve and the deformed angle between two material curves. Given an infinitesimal element of the material curve  $d\mathbf{X} = \mathbf{M}ds$ , its deformed length is  $|d\mathbf{x}| = \sqrt{\mathbf{F}\mathbf{M} \cdot \mathbf{F}\mathbf{M}}ds = \mu ds$  and therefore the deformed length of a material curve with reference arc-length  $s_1 - s_0$  is

$$l_c(t) = \int_{s_0}^{s_1} \mu(s, t) ds. \quad (2.30)$$

Consider two material curves intersecting at  $\mathbf{X}$  with associated unit tangent vectors  $\mathbf{M}_1$  and  $\mathbf{M}_2$ , respectively. Let  $\mu_1$  and  $\mu_2$  be the local stretches corresponding to the two curves and let  $\theta$  be the angle between the tangent vectors of the deformed curve at  $\mathbf{x}$ . We then write,  $\mu_1\mu_2 \cos \theta = \mathbf{F}\mathbf{M}_1 \cdot \mathbf{F}\mathbf{M}_2 = \mathbf{M}_1 \cdot \mathbf{C}\mathbf{M}_2$  and, on using (2.29), obtain

$$\cos \theta = \frac{\mathbf{M}_1 \cdot \mathbf{C}\mathbf{M}_2}{\sqrt{(\mathbf{M}_1 \cdot \mathbf{C}\mathbf{M}_1)(\mathbf{M}_2 \cdot \mathbf{C}\mathbf{M}_2)}}. \quad (2.31)$$

Finally, we introduce two definitions of extensional strain: The first, denoted  $\mathbf{e}_C$  and defined by  $\mathbf{e}_C = \frac{1}{2}(\mathbf{C} - \mathbf{1})$ , yields  $\frac{1}{2}(\mu^2 - 1) = \mathbf{M} \cdot \mathbf{e}_C \mathbf{M}$ , where  $\mathbf{1} \in Lin$  is the identity transformation. Therefore,  $\mathbf{e}_C : \mathcal{V}_\kappa \rightarrow \mathcal{V}_\kappa$  characterizes the relative local stretch with respect to the reference configuration. It is known as the *relative Lagrange strain* or the *Green-St.Venant strain*. Alternatively, to characterize local stretch relative to the current configuration, we define  $\mathbf{e}_B = \frac{1}{2}(\mathbf{1} - \mathbf{B}^{-1})$ , and obtain  $\frac{1}{2}(1 - \mu^{-2}) = \frac{1}{2}\mathbf{m} \cdot (\mathbf{1} - \mathbf{B}^{-1})\mathbf{m}$ . The tensor  $\mathbf{e}_B : \mathcal{V}_\chi \rightarrow \mathcal{V}_\chi$  is called the *relative Eulerian strain* or the *Almansi-Hamel strain tensor*. The two strain tensors are related by  $\mathbf{e}_C = \mathbf{F}^T \mathbf{e}_B \mathbf{F}$ .

Using equations (2.3) and (2.21), we can obtain the deformation gradient from the displacement field,  $\mathbf{F} = \mathbf{1} + \nabla \mathbf{u}$ . For small deformations  $|\nabla \mathbf{u}| \ll 1$  and consequently  $\mu \approx 1$  and  $\mathbf{e}_C \approx \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^T)$  ( $\approx$  denotes the small deformation approximation). The two strain measures are asymptotically coincident in this approximation.

**Principal stretches** We would now like to identify the material curves along which the local stretch assumes extreme values and obtain these extremals from  $\mathbf{C}$ . Define  $f(\mathbf{M}) = \mathbf{M} \cdot \mathbf{C}\mathbf{M}$  at fixed  $\mathbf{C}$ . We therefore have  $f(\mathbf{M}) > 0$  (from (2.29)), for  $\mathbf{M} \in \mathcal{S} = \{\mathbf{v} \in \mathcal{V}_\kappa : |\mathbf{v}| = 1\}$ . Since  $f(\mathbf{M})$  is a continuous function, defined on a compact set, a theorem in analysis ([152],

page 89) yields the existence of  $\mathbf{M}_1 \in \mathcal{S}$  and  $\mathbf{M}_2 \in \mathcal{S}$  such that  $f(\mathbf{M}_1) = \min_{\mathbf{M} \in \mathcal{S}} f(\mathbf{M}) \equiv \lambda_1^2$  and  $f(\mathbf{M}_2) = \max_{\mathbf{M} \in \mathcal{S}} f(\mathbf{M}) \equiv \lambda_2^2$ , respectively. Our aim is to compute  $\lambda_1^2$  and  $\lambda_2^2$  for a given  $\mathbf{C}$ . These are extremal values of  $f(\mathbf{M})$  and thus render  $f(\mathbf{M})$  stationary, i.e.  $df(\mathbf{M}) = 0$ , or  $\mathbf{C}\mathbf{M} \cdot d\mathbf{M} = 0$  for  $\mathbf{M} \in \{\mathbf{M}_1, \mathbf{M}_2\}$ . Furthermore, the identity  $\mathbf{M} \cdot \mathbf{M} = 1$  implies  $\mathbf{M} \cdot d\mathbf{M} = 0$  and therefore  $d\mathbf{M} \perp \mathbf{M}$  at each  $\mathbf{M} \in \mathcal{S}$ . Since  $\mathcal{S}$  is a two dimensional manifold with  $d\mathbf{M}$  belonging to its tangent space, the vector  $\mathbf{M}$  represents the unit vector normal to  $\mathcal{S}$  at  $\mathbf{M} \in \mathcal{S}$ . As a result of these arguments, for some  $\mu_1, \mu_2 \in \mathbb{R}$  we can write,  $\mathbf{C}\mathbf{M}_1 = \mu_1\mathbf{M}_1$  and  $\mathbf{C}\mathbf{M}_2 = \mu_2\mathbf{M}_2$ . Evidently,  $\mu_1$  and  $\mu_2$  are equal to  $\lambda_1^2$  and  $\lambda_2^2$ , respectively ( $\mu_1 = \mathbf{M}_1 \cdot \mathbf{C}\mathbf{M}_1 = f(\mathbf{M}_1) = \lambda_1^2$ , etc.), the largest and smallest eigenvalues of  $\mathbf{C}$ , respectively, and thus,

$$\mathbf{C}\mathbf{M}_1 = \lambda_1^2\mathbf{M}_1, \quad \mathbf{C}\mathbf{M}_2 = \lambda_2^2\mathbf{M}_2. \quad (2.32)$$

In general, for  $\lambda \in \mathbb{R}$  and  $\mathbf{M} \in \mathcal{S}$ , we can solve the eigenvalue problem  $\mathbf{C}\mathbf{M} = \lambda^2\mathbf{M}$  to obtain three real values for  $\lambda^2$ . If  $\{\mathbf{E}_A\}$  is an orthonormal basis for  $\mathcal{V}_\kappa$  and if we set  $C_{AB} = \mathbf{E}_A \cdot \mathbf{C}\mathbf{E}_B$ , then we can conclude that the eigenvalues bound the diagonal entries of the matrix  $\{C_{AB}\}$ ; i.e.

$$\lambda_1^2 \leq \min\{C_{11}, C_{22}, C_{33}\} \leq \max\{C_{11}, C_{22}, C_{33}\} \leq \lambda_2^2. \quad (2.33)$$

**Three theorems for tensors** According to the *spectral theorem*, for  $\mathbf{A} \in \text{Sym}$ , there exists an orthonormal basis  $\{\mathbf{u}_i\} \in \mathcal{V}$  ( $i = 1, 2, 3$ ) and numbers  $\lambda_i \in \mathbb{R}$  such that

$$\mathbf{A} = \sum_{i=1}^3 \lambda_i \mathbf{u}_i \otimes \mathbf{u}_i. \quad (2.34)$$

The numbers  $\lambda_i$  are the principal values associated with the tensor  $\mathbf{A}$  and can be obtained as the roots of the characteristic equation  $\det(\mathbf{A} - \lambda\mathbf{1}) = 0$  with  $\lambda \in \mathbb{R}$ .

According to the *square root theorem*, for every  $\mathbf{A} \in Sym^+$ , there exists a unique tensor  $\mathbf{G} \in Sym^+$  such that  $\mathbf{A} = \mathbf{G}^2$ .

According to the *Polar decomposition theorem*, every  $\mathbf{F} \in InvLin$  can be uniquely decomposed in terms of tensors  $\{\mathbf{U}, \mathbf{V}\} \in Sym^+$  and a rotation  $\mathbf{R} \in Orth^+$  such that

$$\mathbf{F} = \mathbf{R}\mathbf{U} = \mathbf{V}\mathbf{R}. \quad (2.35)$$

A proof of these theorems can be found in [65] among other places.

**Principal invariants** The characteristic equation for  $\mathbf{A} \in Lin$  is

$$0 = \det(\mathbf{A} - \lambda\mathbf{1}) = -\lambda^3 + \lambda^2 I_1(\mathbf{A}) - \lambda I_2(\mathbf{A}) + I_3(\mathbf{A}), \quad (2.36)$$

where

$$\begin{aligned} I_1(\mathbf{A}) &= \text{tr } \mathbf{A} \\ I_2(\mathbf{A}) &= \text{tr } \mathbf{A}^* = \frac{1}{2}[(\text{tr } \mathbf{A})^2 - \text{tr } \mathbf{A}^2] \\ I_3(\mathbf{A}) &= \det \mathbf{A} \end{aligned} \quad (2.37)$$

are the *principal invariants* of  $\mathbf{A}$ . A physically meaningful interpretation of these invariants can be given by identifying  $\mathbf{A}$  with  $\mathbf{U} \in Sym^+$  which appears in the polar decomposition (2.35) of the deformation gradient. In terms of the eigenvalues of  $\mathbf{U}$  (denoted by  $\lambda_i > 0$ ), we obtain from (2.37),  $I_1(\mathbf{U}) = \lambda_1 + \lambda_2 + \lambda_3$ ,  $I_2(\mathbf{U}) = \lambda_1\lambda_2 + \lambda_1\lambda_3 + \lambda_2\lambda_3$  and  $I_3(\mathbf{U}) = \lambda_1\lambda_2\lambda_3$ . Therefore, if the edges of a unit cube are aligned with the eigenvectors of  $\mathbf{U}$ , then  $I_1(\mathbf{U})$  is the sum of the lengths of three mutually orthogonal edges after deformation,  $I_2(\mathbf{U})$  is the sum of the areas of three mutually orthogonal sides after deformation, and  $I_3(\mathbf{U})$  is the deformed volume.

According to the *Cayley-Hamilton theorem*,  $\mathbf{A}$  satisfies its own characteristic equation, i.e.

$$-\mathbf{A}^3 + I_1(\mathbf{A})\mathbf{A}^2 - I_2(\mathbf{A})\mathbf{A} + I_3(\mathbf{A}) = \mathbf{0}. \quad (2.38)$$

We now prove this theorem. Let  $\mathbf{D} = ((\mathbf{A} - \lambda\mathbf{1})^*)^T$ , where  $\lambda \in \mathbb{R}$  is such that  $\det(\mathbf{A} - \lambda\mathbf{1}) \neq 0$  but otherwise arbitrary. Since  $\mathbf{A} - \lambda\mathbf{1}$  is invertible, we have  $\mathbf{D} = \det(\mathbf{A} - \lambda\mathbf{1})(\mathbf{A} - \lambda\mathbf{1})^{-1}$  or  $\mathbf{D}(\mathbf{A} - \lambda\mathbf{1}) = \det(\mathbf{A} - \lambda\mathbf{1})\mathbf{1}$ . The right hand side of this relation is cubic in  $\lambda$  and the term  $\mathbf{A} - \lambda\mathbf{1}$  is linear in  $\lambda$ . Therefore  $\mathbf{D}$  has to be quadratic in  $\lambda$  (by a theorem on factorization of polynomials). Let  $\mathbf{D} = \mathbf{D}_0 + \mathbf{D}_1\lambda + \mathbf{D}_2\lambda^2$  for some  $\mathbf{D}_0$ ,  $\mathbf{D}_1$  and  $\mathbf{D}_2$ . Then  $(\mathbf{D}_0 + \mathbf{D}_1\lambda + \mathbf{D}_2\lambda^2)(\mathbf{A} - \lambda\mathbf{1}) = \det(\mathbf{A} - \lambda\mathbf{1})\mathbf{1} = (-\lambda^3 + \lambda^2 I_1 - \lambda I_2 + I_3)\mathbf{1}$ . Matching coefficients of various powers of  $\lambda$  between the first and the last term and eliminating  $\mathbf{D}_0$ ,  $\mathbf{D}_1$  and  $\mathbf{D}_2$  from these, we get the required relation (2.38). The coefficients of all the powers of  $\lambda$  have to vanish since otherwise we would obtain a polynomial (of order 3) in  $\lambda$ , which could then be solved to obtain roots for  $\lambda$ , contradicting the premise that  $\lambda \in \mathbb{R}$  is arbitrary.

**Velocity gradient** We can use the chain rule for differentiation to write the gradient of the velocity field with respect to  $\mathbf{X}$  as

$$\nabla \hat{\mathbf{v}}(\mathbf{X}, t) = \mathbf{L}\mathbf{F}, \quad (2.39)$$

where  $\mathbf{L} = \text{grad } \tilde{\mathbf{v}} : \mathcal{V}_\chi \rightarrow \mathcal{V}_\chi$  is the *spatial velocity gradient*. Under sufficient continuity of the motion we have  $\nabla \hat{\mathbf{v}} = \dot{\mathbf{F}}$  and therefore  $\mathbf{L} = \dot{\mathbf{F}}\mathbf{F}^{-1}$ . We can decompose  $\mathbf{L}$  into  $\mathbf{D} \in \text{Sym}$  (*rate of deformation tensor*) and  $\mathbf{W} \in \text{Skw}$  (*vorticity tensor*). The material time derivative of the right and the left Cauchy-Green tensor can be obtained as

$$\dot{\mathbf{C}} = 2\mathbf{F}^T \mathbf{D} \mathbf{F}, \quad \dot{\mathbf{B}} = \mathbf{L}\mathbf{B} + \mathbf{B}\mathbf{L}^T. \quad (2.40)$$

Indeed,  $\dot{\mathbf{C}} = \dot{\mathbf{F}}^T \mathbf{F} + \mathbf{F}^T \dot{\mathbf{F}} = \mathbf{F}^T \mathbf{L}^T \mathbf{F} + \mathbf{F}^T \mathbf{L} \mathbf{F}$  and  $\dot{\mathbf{B}} = \dot{\mathbf{F}} \mathbf{F}^T + \mathbf{F} \dot{\mathbf{F}}^T = \mathbf{L} \mathbf{F} \mathbf{F}^T + \mathbf{F} \mathbf{F}^T \mathbf{L}^T$ .

For a fixed material curve with unit tangent vector  $\mathbf{M}$  recall relation (2.28), i.e.  $\mu \mathbf{m} = \mathbf{F} \mathbf{M}$ . As a result

$$\frac{\dot{\mu}}{\mu} = \mathbf{m} \cdot \mathbf{D} \mathbf{m}, \quad (2.41)$$

where we have used  $\dot{\mathbf{M}} = 0$ ,  $\mathbf{m} \cdot \dot{\mathbf{m}} = 0$  (which follows from  $\mathbf{m} \cdot \mathbf{m} = 1$ ) and  $\mathbf{m} \cdot \mathbf{W} \mathbf{m} = 0$  (since  $\mathbf{m} \cdot \mathbf{W} \mathbf{m} = \mathbf{W}^T \mathbf{m} \cdot \mathbf{m} = -\mathbf{W} \mathbf{m} \cdot \mathbf{m}$ ). We also obtain  $\mu \dot{\mathbf{m}} = \mu \mathbf{L} \mathbf{m} - \dot{\mu} \mathbf{m}$ , which on using (2.41) and the decomposition of  $\mathbf{L}$  into symmetric and skew parts, reduces to

$$\dot{\mathbf{m}} = \mathbf{D} \mathbf{m} - (\mathbf{m} \cdot \mathbf{D} \mathbf{m}) \mathbf{m} + \mathbf{W} \mathbf{m}. \quad (2.42)$$

If  $\mathbf{m}$  should coincide with a principal vector of  $\mathbf{D}$  with principal value  $\gamma$ , then  $\mathbf{D} \mathbf{m} = \gamma \mathbf{m}$ . The relations (2.41) and (2.42) in this case give  $\gamma = \frac{\dot{\mu}}{\mu} = (\ln \mu)'$  and  $\dot{\mathbf{m}} = \mathbf{W} \mathbf{m}$ , respectively. Therefore, when the unit tangent  $\mathbf{m}$  to the deformed material curve instantaneously aligns with a principal vector of  $\mathbf{D}$ , the corresponding principal value of  $\mathbf{D}$  is the rate of the natural logarithm of the stretch associated with the material curve. Moreover, the vorticity tensor  $\mathbf{W}$  then characterizes the spin of the material element instantaneously aligned with a principal vector.

Associated with  $\mathbf{W} \in Skw$  there exists a vector  $\mathbf{w} \in \mathcal{V}_\chi$  (the axial vector of  $\mathbf{W}$ ) such that,  $\mathbf{W} \mathbf{a} = \mathbf{w} \times \mathbf{a}$  for all  $\mathbf{a} \in \mathcal{V}_\chi$ . This fact can be proved by first obtaining the canonical form for a skew tensor. The characteristic equation for  $\mathbf{W}$  has three roots and therefore at least one of them is real (complex roots occur in a pair). Let this real eigenvalue be  $\lambda$  and let  $\mathbf{f} \in \mathcal{V}_\chi$  be the corresponding eigenvector. Then  $\mathbf{W} \mathbf{f} = \lambda \mathbf{f}$ . But this implies  $\lambda = \mathbf{W} \mathbf{f} \cdot \mathbf{f} = 0$  and so  $\mathbf{W} \mathbf{f} = 0$ . Choose  $\{\mathbf{g}, \mathbf{h}\} \in \mathcal{V}_\chi$  such that  $\{\mathbf{f}, \mathbf{g}, \mathbf{h}\}$  forms a right

handed orthonormal basis for  $\mathcal{V}_\chi$ . The canonical form for  $\mathbf{W}$  is then given by

$$\mathbf{W} = \omega(\mathbf{h} \otimes \mathbf{g} - \mathbf{g} \otimes \mathbf{h}), \quad (2.43)$$

where  $\omega = \mathbf{h} \cdot \mathbf{W}\mathbf{g}$ . The canonical form (2.43) can be proved by remembering that  $\mathbf{W}^T = -\mathbf{W}$ ,  $\mathbf{W}\mathbf{f} = \mathbf{0}$  and  $\mathbf{a} \cdot \mathbf{W}\mathbf{a} = 0$  for all  $\mathbf{a} \in \mathcal{V}_\chi$ . Then  $\mathbf{W} = \mathbf{W}\mathbf{I} = \mathbf{W}(\mathbf{f} \otimes \mathbf{f} + \mathbf{g} \otimes \mathbf{g} + \mathbf{h} \otimes \mathbf{h}) = \mathbf{W}\mathbf{g} \otimes \mathbf{g} + \mathbf{W}\mathbf{h} \otimes \mathbf{h}$ . Note that  $\mathbf{W}\mathbf{g} = \omega\mathbf{h}$ , since  $\mathbf{W}\mathbf{g} \cdot \mathbf{f} = -\mathbf{g} \cdot \mathbf{W}\mathbf{f} = 0$  and  $\mathbf{W}\mathbf{g} \cdot \mathbf{g} = 0$ . Similarly  $\mathbf{W}\mathbf{h} = -\omega\mathbf{g}$ . This completes the proof.

Let  $\mathbf{w} = \omega\mathbf{f}$ . Then on using (2.43) for arbitrary  $\mathbf{a}$ , we obtain  $\mathbf{W}\mathbf{a} = \omega((\mathbf{g} \cdot \mathbf{a})\mathbf{h} - (\mathbf{h} \cdot \mathbf{a})\mathbf{g}) = \omega((\mathbf{g} \cdot \mathbf{a})(\mathbf{f} \times \mathbf{g}) - (\mathbf{h} \cdot \mathbf{a})(\mathbf{h} \times \mathbf{f})) = \omega\mathbf{f} \times ((\mathbf{f} \cdot \mathbf{a})\mathbf{f} + (\mathbf{g} \cdot \mathbf{a})\mathbf{g} + (\mathbf{h} \cdot \mathbf{a})\mathbf{h}) = \mathbf{w} \times \mathbf{a}$ .

If  $\mathbf{W}$  is the skew part of the spatial velocity gradient, then the axial vector  $\mathbf{w}$  is given in terms of the velocity field  $\mathbf{v}$  by

$$\mathbf{w} = \frac{1}{2} \text{curl } \tilde{\mathbf{v}}. \quad (2.44)$$

The vector  $\mathbf{w}$  is also called the vorticity vector. This relation can be proved by considering two constant but otherwise arbitrary vectors  $\mathbf{g}$  and  $\mathbf{h}$ . Therefore  $2\mathbf{W}\mathbf{g} \cdot \mathbf{h} = ((\text{grad } \tilde{\mathbf{v}}) - (\text{grad } \tilde{\mathbf{v}})^T)\mathbf{g} \cdot \mathbf{h} = \text{div}((\tilde{\mathbf{v}} \cdot \mathbf{h})\mathbf{g} - (\tilde{\mathbf{v}} \cdot \mathbf{g})\mathbf{h}) = \text{div}(\tilde{\mathbf{v}} \times (\mathbf{g} \times \mathbf{h})) = \text{curl } \tilde{\mathbf{v}} \cdot \mathbf{g} \times \mathbf{h} = (\text{curl } \tilde{\mathbf{v}} \times \mathbf{g}) \cdot \mathbf{h}$ . Using the arbitrariness of  $\mathbf{h}$  and the relation  $\mathbf{W}\mathbf{g} = \mathbf{w} \times \mathbf{g}$  we obtain equation (2.44).

Finally, we interpret the off-diagonal terms of  $\mathbf{D}$  on an orthogonal basis. Consider two intersecting material curves with tangent vectors  $\mathbf{M}_1$  and  $\mathbf{M}_2$  at the point of intersection. In the current configuration, they map to  $\mathbf{m}_1$  and  $\mathbf{m}_2$  with local stretches  $\mu_1$  and  $\mu_2$ , respectively. Let  $\cos \theta = \mathbf{m}_1 \cdot \mathbf{m}_2$ . Then,  $(\sin \theta)\dot{\theta} = (\mathbf{m}_1 \cdot \mathbf{D}\mathbf{m}_1 + \mathbf{m}_2 \cdot \mathbf{D}\mathbf{m}_2)(\mathbf{m}_1 \cdot \mathbf{m}_2) - 2\mathbf{m}_1 \cdot \mathbf{D}\mathbf{m}_2$ , where relation (2.42) has been used. If  $\sin \theta = 1$  (i.e.  $\mathbf{m}_1 \cdot \mathbf{m}_2 = 0$ ), we have  $\dot{\theta} = -2\mathbf{m}_1 \cdot \mathbf{D}\mathbf{m}_2$ . Therefore the off-diagonal terms of  $\mathbf{D}$  on an orthogonal basis are



proportional to the rate of change of the angle between tangents to the deformed material curves instantaneously aligned with the orthogonal elements of the basis.

#### 2.1.4 Singular surfaces

By a singular surface, we refer to a surface in the body across which jump discontinuities are allowed for various fields (and their derivatives) which otherwise are continuous in the body. The jump of a field (say  $\Psi$ ) across a singular surface is denoted by

$$[[\Psi]] = \Psi^+ - \Psi^-, \quad (2.45)$$

where  $\Psi^+$  and  $\Psi^-$  are the limit values of  $\Psi$  as it approaches the singular surface from either side. The ‘+’ side is taken to be the one into which the normal to the surface points. Let  $\Phi$  be another piecewise continuous field. The following relation, which can be verified by direct substitution using (2.45), will find much use in our later developments

$$[[\Phi\Psi]] = [[\Phi]]\langle\Psi\rangle + \langle\Phi\rangle[[\Psi]], \quad (2.46)$$

where

$$\langle\Psi\rangle = \frac{\Psi^+ + \Psi^-}{2}. \quad (2.47)$$

A two dimensional surface which evolves in time is given by

$$S_t = \{\mathbf{X} \in \kappa(\mathfrak{B}) : \phi(\mathbf{X}, t) = 0\}, \quad (2.48)$$

where  $\phi : \kappa(\mathfrak{B}) \times \mathbb{R} \rightarrow \mathbb{R}$  is a continuously differentiable function. The referential normal to the surface and the referential normal velocity are defined by

$$\begin{aligned} \mathbf{N}(\mathbf{X}, t) &= \frac{\nabla\phi}{|\nabla\phi|} \quad \text{and} \\ U(\mathbf{X}, t) &= -\frac{\dot{\phi}}{|\nabla\phi|}, \end{aligned} \quad (2.49)$$

respectively. The second of these definitions is motivated towards the end of this section.

An immediate consequence of these definitions is

$$\dot{\mathbf{N}} = -(\mathbf{1} - \mathbf{N} \otimes \mathbf{N})\nabla U - U(\nabla \mathbf{N})\mathbf{N}. \quad (2.50)$$

Indeed, we have from (2.49)<sub>1</sub>

$$\dot{\mathbf{N}} = \frac{\nabla \dot{\phi}}{|\nabla \phi|} - \frac{\nabla \phi}{|\nabla \phi|^2} \left( \frac{\nabla \phi}{|\nabla \phi|} \cdot \nabla \dot{\phi} \right) = \frac{\nabla \dot{\phi}}{|\nabla \phi|} (\mathbf{1} - \mathbf{N} \otimes \mathbf{N}) \quad \text{and} \quad (2.51)$$

$$\nabla \mathbf{N} = \frac{\nabla^2 \phi}{|\nabla \phi|} - \frac{\nabla \phi}{|\nabla \phi|^2} \otimes \left( \nabla^2 \phi \frac{\nabla \phi}{|\nabla \phi|} \right) = \frac{\nabla^2 \phi}{|\nabla \phi|} - \mathbf{N} \otimes \frac{(\nabla^2 \phi)\mathbf{N}}{|\nabla \phi|}. \quad (2.52)$$

On the other hand, (2.49)<sub>2</sub> yields

$$\nabla U = -\frac{\nabla \dot{\phi}}{|\nabla \phi|} + \frac{\dot{\phi}}{|\nabla \phi|^2} \left( \nabla^2 \phi \frac{\nabla \phi}{|\nabla \phi|} \right) = -\frac{\nabla \dot{\phi}}{|\nabla \phi|} - U \frac{(\nabla^2 \phi)\mathbf{N}}{|\nabla \phi|}, \quad (2.53)$$

where  $\nabla^2 \phi = \nabla(\nabla \phi) \in Sym$ . Combining these relations we obtain (2.50). The tensor  $\mathbf{1} - \mathbf{N} \otimes \mathbf{N}$  is the orthogonal projection onto  $\mathcal{V}_\kappa$  and is denoted by  $\mathbb{P}$ . It is easy to check that  $\mathbb{P}^T = \mathbb{P}$  and  $\mathbb{P}\mathbb{P} = \mathbb{P}$ .

**Derivatives** We now define surface derivatives for scalar, vector and tensor valued functions which are defined on the surface  $S_t$ . Let  $f$  denote a scalar, vector or tensor valued function on  $S_t$ . The function  $f$  is differentiable at  $\mathbf{X} \in S_t$  if  $f$  has an extension  $f$  to a neighborhood  $N$  of  $\mathbf{X}$ , which is differentiable at  $\mathbf{X}$  in the classical sense (see subsection 2.1.2) and is equal to  $f$  for  $\mathbf{X} \in S_t$ . The *surface gradient* of  $f$  at  $\mathbf{X} \in S_t$  is then defined by

$$\nabla^S f(\mathbf{X}) = \nabla f(\mathbf{X})\mathbb{P}(\mathbf{X}). \quad (2.54)$$

Let  $\mathbf{v} : S_t \rightarrow \mathcal{V}$  and  $\mathbf{A} : S_t \rightarrow Lin$  be respectively, vector and tensor valued functions on the surface  $S_t$ . We define the *surface divergence* as a scalar field  $\text{Div}^S \mathbf{v}$  and a vector field

$\text{Div}^S A$  by

$$\begin{aligned} \text{Div}^S v &= \text{tr}(\nabla^S v) \\ \mathbf{c} \cdot \text{Div}^S A &= \text{Div}^S(A^T \mathbf{c}) \end{aligned} \quad (2.55)$$

for any fixed  $\mathbf{c} \in \mathcal{V}$ . Moreover, we call  $v$  *tangential* if  $\mathbb{P}v = v$  and  $A$  *superficial* if  $A\mathbb{P} = A$ .

We define the *curvature tensor*  $L$  by<sup>2</sup>

$$L = -\nabla^S \mathbf{N}, \quad (2.56)$$

or  $L = -\nabla \mathbf{N}(\mathbf{1} - \mathbf{N} \otimes \mathbf{N})$ . Therefore

$$\text{tr} L = -\text{Div} \mathbf{N} + (\nabla \mathbf{N}) \mathbf{N} \cdot \mathbf{N} = -\text{Div} \mathbf{N}, \quad (2.57)$$

where we have used  $(\nabla \mathbf{N})^T \mathbf{N} = \mathbf{0}$ , which follows from  $\mathbf{N} \cdot \mathbf{N} = 1$ . Since  $\nabla^S \mathbf{N} \mathbb{P} = \nabla \mathbf{N} \mathbb{P} \mathbb{P} = \nabla \mathbf{N} \mathbb{P} = \nabla^S \mathbf{N}$ , the curvature tensor is superficial. Furthermore, using (2.52) we have

$$\begin{aligned} L &= -\nabla \mathbf{N}(\mathbf{1} - \mathbf{N} \otimes \mathbf{N}) \\ &= -\left( \frac{\nabla^2 \phi}{|\nabla \phi|} - \mathbf{N} \otimes \frac{(\nabla^2 \phi) \mathbf{N}}{|\nabla \phi|} \right) (\mathbf{1} - \mathbf{N} \otimes \mathbf{N}) \\ &= \frac{-1}{|\nabla \phi|} \{ \nabla^2 \phi - \mathbf{N} \otimes (\nabla^2 \phi) \mathbf{N} - (\nabla^2 \phi) \mathbf{N} \otimes \mathbf{N} + ((\nabla^2 \phi) \mathbf{N} \cdot \mathbf{N}) \mathbf{N} \otimes \mathbf{N} \} \end{aligned}$$

and consequently we infer that  $L = L^T$  and  $L\mathbf{N} = \mathbf{0}$ . Therefore,  $\mathbf{N}$  is a principal direction of  $L$  with the corresponding principal value being zero. Since  $L$  is symmetric, the spectral theorem implies that it has three real eigenvalues with mutually orthogonal eigenvectors.

We have already obtained zero as an eigenvalue (with  $\mathbf{N}$  as the eigenvector). Let the other

---

<sup>2</sup>The normal  $\mathbf{N}$  and its extension to a neighborhood of  $S_t$  are both denoted by the same symbol. See Remark 2.1.1.

eigenvalues be  $\kappa_1$  and  $\kappa_2$ , whose corresponding eigenvectors lie in the plane normal to  $\mathbf{N}$ .

The mean and the Gaussian curvature associated with the surface are then defined as

$$H = \frac{1}{2}(\kappa_1 + \kappa_2), \quad \text{and } K = \kappa_1\kappa_2, \quad (2.58)$$

respectively.

A function  $\varphi : (t - \varepsilon, t + \varepsilon) \rightarrow \mathcal{E}_\kappa$ ,  $\varepsilon > 0$ , is said to be a *normal curve* through  $\mathbf{X} \in S_t$  at time  $t$  if for each  $\tau \in (t - \varepsilon, t + \varepsilon)$ ,

$$\varphi'(\tau) = U(\varphi(\tau), \tau)\mathbf{N}(\varphi(\tau), \tau). \quad (2.59)$$

The function  $\varphi(\tau)$  is therefore the position parameterized by  $\tau$ . We define the *normal time derivative* of a function on  $S_t$  by

$$\dot{\varphi}(\mathbf{X}, t) = \left. \frac{d\varphi(\varphi(\tau), \tau)}{d\tau} \right|_{\tau=t}. \quad (2.60)$$

The relation (2.50) can therefore be written as  $\dot{\mathbf{N}} = -\nabla^S U$ .

*Remark 2.1.1.* We will assume that an extension of a surface field to a neighborhood of the surface exists, and will abuse the notation to use the same symbol for the field and its extension.

**Compatibility conditions** Central to the discussion on the kinematics of singular surfaces are the compatibility conditions which relate the deformation gradient and the velocity field across the singular surface. Consider a closed material curve  $C \subset \mathcal{E}_\kappa$  such that it intersects the singular surface  $S_t$  at two points, say  $\mathbf{p}_1$  and  $\mathbf{p}_2$ . Let  $A_C$  be the area bounded by  $C$  and let  $\Gamma = A_C \cap S_t$  be the line of intersection of this area with the singular surface. We parameterize  $\Gamma$  by arc-length  $u$  such that the curve  $\Gamma$  extends from  $\mathbf{p}_2$  to  $\mathbf{p}_1$ .

In general we can write

$$\mathbf{b} = \oint_C \mathbf{F} d\mathbf{X}, \quad (2.61)$$

where a non-zero  $\mathbf{b} \in \mathcal{E}_\chi$  arises when  $\mathbf{F}$  is incompatible (we assume for now that  $\mathbf{F}$  is not expressible as a gradient). In dislocation theory  $\mathbf{b}$  is referred to as the Burgers vector associated with the closed curve  $C$ . The integration in the above relation is well defined since we assume  $\mathbf{F}$  to be singular only over a set of zero Lebesgue measure (a finite number of points on a continuous line constitute such a set). According to Stokes' theorem with a singular surface,

$$\mathbf{b} = \oint_C \mathbf{F} d\mathbf{X} = \int_{A_C} (\text{Curl } \mathbf{F})^T \mathbf{N}_A dA - \int_\Gamma \llbracket \mathbf{F} \rrbracket d\mathbf{X}, \quad (2.62)$$

where  $\mathbf{N}_A$  is the unit normal associated with the area  $A_C$ . A proof of this theorem is given in subsection 2.2.1 (cf. (2.102)). We discuss two consequences of the above relation:

(i) Let  $\mathbf{b} = \mathbf{0}$ . Then,  $\text{Curl } \mathbf{F} = \mathbf{0}$  in  $\kappa(\mathfrak{B}) \setminus S_t$ . We can show this by choosing a  $C$  such that  $\Gamma = \emptyset$ . The arbitrariness of  $A_C$  (and thus of  $\mathbf{N}_A$ ) and the localization theorem for surface integrals (see subsection 2.2.1) then imply  $\text{Curl } \mathbf{F} = \mathbf{0}$  for all  $\mathbf{X} \in \kappa(\mathfrak{B}) \setminus S_t$ . Equation (2.62) now reduces to

$$\mathbf{0} = \int_\Gamma \llbracket \mathbf{F} \rrbracket d\mathbf{X}. \quad (2.63)$$

Use the parametrization of  $\Gamma$  to write  $d\mathbf{X} = sdu$ , where  $\mathbf{s} \in T_{S_t(\mathbf{X})}$  is a unit vector in the tangent plane  $T_{S_t(\mathbf{X})}$  to  $S_t$  at  $\mathbf{X}$ . The curve  $C$  can be arbitrarily chosen and therefore  $\Gamma$  is arbitrary. Use the arbitrariness of  $\Gamma$  to localize (2.63), and obtain

$$\llbracket \mathbf{F} \rrbracket \mathbf{s} = \mathbf{0} \quad (2.64)$$

for all  $\mathbf{s} \in T_{S_t(\mathbf{X})}$ . Thus, there exists a vector  $\mathbf{k} \in \mathcal{V}_\chi$  such that

$$[[\mathbf{F}]] = \mathbf{k} \otimes \mathbf{N} \quad (2.65)$$

on  $S_t$ , which is *Hadamard's compatibility condition* for the deformation gradient.

(ii) Let  $\text{Curl } \mathbf{F} = \mathbf{0}$  in  $\kappa(\mathfrak{B}) \setminus S_t$ . Therefore there exists a vector field  $\chi_\kappa$  such that  $\mathbf{F} = \nabla \chi_\kappa$  away from  $S_t$ . Note that  $\chi_\kappa$  might still suffer a jump across  $S_t$ . Let  $C^+ \cup C^- = C$ , where  $C^+$  and  $C^-$  are two disjoint parts of  $C$  which lie on the '+' and '-' side of  $S_t$ , respectively. The '+' side is the one into which the normal  $\mathbf{N}$  points. Therefore,

$$\begin{aligned} \oint_C \mathbf{F} d\mathbf{X} &= \int_{C^+} \mathbf{F} d\mathbf{X} + \int_{C^-} \mathbf{F} d\mathbf{X} \\ &= \chi_2^+ - \chi_1^+ + \chi_1^- - \chi_2^- \\ &= [[\chi_\kappa]]_2 - [[\chi_\kappa]]_1 = - \int_\Gamma [[\chi_\kappa]]'(u) du, \end{aligned} \quad (2.66)$$

where  $\chi_2^+ = \chi_\kappa^+(\mathbf{p}_2)$  etc. The negative sign in the last term above arises due to the orientation of  $\Gamma$ , which extends from  $\mathbf{p}_2$  to  $\mathbf{p}_1$ . On the other hand we have in this case, from (2.62),

$$\oint_C \mathbf{F} d\mathbf{X} = - \int_\Gamma [[\mathbf{F}]] d\mathbf{X}. \quad (2.67)$$

Since  $[[\chi_\kappa]]'(u) = \nabla [[\chi_\kappa]] \mathbf{s} = \nabla^S [[\chi_\kappa]] \mathbf{s}$  (as  $\mathbb{P} \mathbf{s} = \mathbf{s}$ ), we obtain, on comparing equations (2.66) and (2.67) and using the arbitrariness of  $\Gamma$

$$[[\mathbf{F}]] \mathbf{s} = \nabla^S [[\chi_\kappa]] \mathbf{s} \quad (2.68)$$

for all  $\mathbf{s} \in T_{S_t(\mathbf{X})}$ . Thus, there exists a vector  $\mathbf{k} \in \mathcal{E}_\chi$  such that

$$[[\mathbf{F}]] = \mathbf{k} \otimes \mathbf{N} + \nabla^S [[\chi_\kappa]] \quad (2.69)$$

on  $S_t$ , which is the modified compatibility condition for the deformation gradient in the case when  $\boldsymbol{\chi}_\kappa$  suffers a jump on the singular surface. If  $[[\boldsymbol{\chi}_\kappa]] = \text{const.}$  then equation (2.69) reduces to Hadamard's compatibility condition (2.65).

To obtain the compatibility condition for the velocity field, we apply the definition of the normal time derivative (cf. (2.59), (2.60)) on fields  $\boldsymbol{\chi}_\kappa^+$  and  $\boldsymbol{\chi}_\kappa^-$ . We obtain

$$(\boldsymbol{\chi}_\kappa^+)^{\circ} = \left. \frac{d\boldsymbol{\chi}_\kappa(\boldsymbol{\varphi}(\tau), \tau)}{d\tau} \right|_{\tau=t^+} = U\mathbf{F}^+\mathbf{N} + \mathbf{v}^+ \quad (2.70)$$

and

$$(\boldsymbol{\chi}_\kappa^-)^{\circ} = \left. \frac{d\boldsymbol{\chi}_\kappa(\boldsymbol{\varphi}(\tau), \tau)}{d\tau} \right|_{\tau=t^-} = U\mathbf{F}^-\mathbf{N} + \mathbf{v}^-, \quad (2.71)$$

where  $\tau \in (t, t + \varepsilon)$  in (2.70) and  $\tau \in (t - \varepsilon, t)$  in (2.71). Subtracting these relations we get the compatibility condition for the velocity field,

$$[[\mathbf{v}]] + U[[\mathbf{F}]]\mathbf{N} = [[\boldsymbol{\chi}_\kappa]]. \quad (2.72)$$

For  $[[\boldsymbol{\chi}_\kappa]] = \text{const.}$  (including the case when  $\boldsymbol{\chi}_\kappa$  is continuous, i.e.  $[[\boldsymbol{\chi}_\kappa]] = \mathbf{0}$ ) this condition reduces to

$$[[\mathbf{v}]] + U[[\mathbf{F}]]\mathbf{N} = \mathbf{0} \quad (2.73)$$

or equivalently

$$U[[\mathbf{F}]] = -[[\mathbf{v}]] \otimes \mathbf{N}. \quad (2.74)$$

**Surface deformation gradient** For a continuous motion across the surface  $S_t$ , we have  $[[\boldsymbol{\chi}_\kappa(\mathbf{X}, t)]] = \mathbf{0}$  for  $\mathbf{X} \in S_t$ , and in this case we can define the *surface deformation gradient*  $\mathbf{F}$  and the *surface normal velocity*  $\mathbf{v}$  by

$$\mathbf{F} = \nabla^S \boldsymbol{\chi}_\kappa, \quad \mathbf{v} = \dot{\boldsymbol{\chi}}_\kappa. \quad (2.75)$$

It is then easy to check that

$$\mathbf{F} = \mathbf{F}^\pm \mathbb{P}, \quad \mathbf{v} = \hat{\mathbf{v}}^\pm + U \mathbf{F}^\pm \mathbf{N}, \quad (2.76)$$

where on the right hand side above,  $\pm$  indicates that either  $+$  or  $-$  can be used, a fact which can be verified using the compatibility conditions (2.65) and (2.73).

The tensor  $\mathbf{F}$  as defined above satisfies  $\det \mathbf{F} = 0$  and  $\mathbf{F}^* \neq \mathbf{0}$ . That  $\det \mathbf{F} = 0$  can be verified using (2.76)<sub>1</sub> and  $\det \mathbb{P} = 0$ . The cofactor  $\mathbf{F}^*$  of  $\mathbf{F}$  is defined by  $\mathbf{F}^*(\mathbf{a} \times \mathbf{b}) = \mathbf{F}\mathbf{a} \times \mathbf{F}\mathbf{b}$  for arbitrary vectors  $\{\mathbf{a}, \mathbf{b}\} \in \mathcal{V}_\kappa$ . Let  $\{\mathbf{t}_1, \mathbf{t}_2\} \in T_{S_t(\mathbf{X})}$  be two unit vectors in the tangent plane to  $S_t$  at  $\mathbf{X} \in S_t$ , such that  $\{\mathbf{t}_1, \mathbf{t}_2, \mathbf{N}\}$  form an orthonormal basis at  $\mathbf{X}$ . Then,

$$\begin{aligned} \mathbf{F}^* \mathbf{N} &= \mathbf{F}^*(\mathbf{t}_1 \times \mathbf{t}_2) = \mathbf{F}\mathbf{t}_1 \times \mathbf{F}\mathbf{t}_2 \\ &= \mathbf{F}^\pm \mathbf{t}_1 \times \mathbf{F}^\pm \mathbf{t}_2 \\ &= (\mathbf{F}^\pm)^* \mathbf{N}, \end{aligned} \quad (2.77)$$

where in the second equality, relation (2.76)<sub>1</sub> has been used. Furthermore, it is straightforward to check that  $\mathbf{F}^* \mathbf{t}_\alpha = \mathbf{0}$  ( $\alpha = 1, 2$ ), since  $\mathbf{F}\mathbf{N} = \mathbf{0}$ . Therefore  $\mathbf{F}^*$  remains non-zero as long as  $(\mathbf{F}^\pm)^* \mathbf{N}$  does not vanish. Note that  $|\mathbf{F}^* \mathbf{N}|$  is equal to the ratio of the infinitesimal areas (on the singular surface) in the current and the reference configuration. This follows immediately from equations (2.24) and (2.77).

**Surface parametrization** Consider  $\mathbf{X} \in \mathcal{E}_\kappa$  in a neighborhood of  $S_t$ . We can then find a point  $\hat{\mathbf{X}} \in S_t$  such that

$$\mathbf{X} = \hat{\mathbf{X}} + \zeta \mathbf{N}, \quad (2.78)$$

where  $\zeta(t) \in \mathbb{R}$  is a scalar. We parameterize the surface  $S_t$  by using a local coordinate system  $(\xi_1, \xi_2)$ , where  $\{\xi_1, \xi_2\} \in \mathbb{R}$ . In terms of the new variables,  $\mathbf{X} = \mathbf{X}(\xi_1, \xi_2, \zeta)$ ,  $\hat{\mathbf{X}} = \hat{\mathbf{X}}(\xi_1, \xi_2, t)$



and  $\mathbf{N} = \hat{\mathbf{N}}(\xi_1, \xi_2, t)$ . Let  $\hat{\mathbf{X}}_{,\alpha} = \boldsymbol{\xi}_\alpha$  for  $\alpha = 1, 2$ . We assume that the parametrization is such that the triad  $\{\boldsymbol{\xi}_1, \boldsymbol{\xi}_2, \mathbf{N}\}$  forms an orthonormal basis at  $\hat{\mathbf{X}}$ . In a sufficiently small neighborhood of  $\mathbf{X} = \mathbf{X}(\xi_1, \xi_2, \zeta)$  it is possible to invert this to obtain  $\boldsymbol{\xi} \equiv (\xi_1, \xi_2, \zeta) = \boldsymbol{\xi}(\mathbf{X})$ .

Use (2.78) to obtain the differential of  $\mathbf{X}$ ,

$$d\mathbf{X} = (\boldsymbol{\xi}_\alpha + \zeta \mathbf{N}_{,\alpha}) d\xi_\alpha + \mathbf{N} d\zeta. \quad (2.79)$$

If we identify with  $\boldsymbol{\xi}_1$  and  $\boldsymbol{\xi}_2$ , the principal directions of  $L$  (recall that  $\mathbf{N}$  is the third principal direction, cf. (2.56) and the paragraph preceding (2.58)), we have  $\mathbf{N}_{,\alpha} = -\kappa_\alpha \boldsymbol{\xi}_\alpha$  (no summation implied over  $\alpha$ ), where  $\kappa_\alpha$  are the principal curvatures associated with the surface. Therefore, if  $\mathbf{A}$  is the gradient of the map taking  $\boldsymbol{\xi}$  to  $\mathbf{X}$  then  $d\mathbf{X} = \mathbf{A} d\boldsymbol{\xi}$  and it follows from (2.79) that

$$\mathbf{A} = \xi_{11}(1 - \kappa_1 \zeta) \boldsymbol{\xi}_1 \otimes \boldsymbol{\xi}_1 + \xi_{22}(1 - \kappa_2 \zeta) \boldsymbol{\xi}_2 \otimes \boldsymbol{\xi}_2 + \mathbf{N} \otimes \mathbf{N}, \quad (2.80)$$

where  $\xi_{\alpha\alpha} = \boldsymbol{\xi}_\alpha \cdot \boldsymbol{\xi}_\alpha$  (no summation). Let  $\xi = \xi_{11}\xi_{22}$ . Thus

$$j_A \equiv \det \mathbf{A} = \xi(1 - 2\zeta H + \zeta^2 K), \quad (2.81)$$

where  $H$  and  $K$  are defined in (2.58).

Taking the differential of the function  $\phi$ ,  $d\phi = \nabla\phi \cdot d\mathbf{X} + \dot{\phi} dt$ , and substituting in it the expression for  $d\mathbf{X}$  from (2.79) for a point near the surface, we obtain

$$d\phi = \nabla\phi \cdot ((\boldsymbol{\xi}_\alpha + \zeta \mathbf{N}_{,\alpha}) d\xi_\alpha + \mathbf{N} d\zeta) + \dot{\phi} dt. \quad (2.82)$$

On the surface, we have  $\zeta = 0$  and  $d\phi = 0$ . Consequently we obtain

$$\begin{aligned} 0 &= \nabla\phi \cdot \boldsymbol{\xi}_\alpha d\xi_\alpha + \nabla\phi \cdot \mathbf{N} d\zeta + \dot{\phi} dt \\ &= \nabla\phi \cdot \boldsymbol{\xi}_\alpha d\xi_\alpha + \nabla\phi \cdot \mathbf{N} \dot{\zeta} dt + \dot{\phi} dt \end{aligned} \quad (2.83)$$

on  $S_t$ , and noting the independence of  $d\xi_\alpha$  and  $dt$ , we recover relations (2.49) along with the identification of  $\dot{\zeta}$  with  $U$ .

**Singular surface in the current configuration** The image of the singular surface  $S_t$  in the current configuration is give by

$$\begin{aligned} s_t = \chi_\kappa(S_t, t) &= \{\mathbf{x} \in \chi(\mathfrak{B}) : \psi(\mathbf{x}, t) = 0\}, \quad \text{where} \\ \psi(\chi_\kappa(\mathbf{X}, t), t) &= \phi(\mathbf{X}, t). \end{aligned} \quad (2.84)$$

The scalar function  $\psi : \chi(\mathfrak{B}) \times \mathbb{R} \rightarrow \mathbb{R}$  is assumed to be continuously differentiable with respect to its arguments. The normal to the surface  $s_t$  and the spatial normal velocity are defined by (cf. (2.49))

$$\begin{aligned} \mathbf{n} &= \frac{\text{grad } \psi}{|\text{grad } \psi|}, \quad \text{and} \\ u &= -\frac{1}{|\text{grad } \psi|} \frac{\partial \psi}{\partial t}, \end{aligned} \quad (2.85)$$

respectively, where  $\frac{\partial \psi}{\partial t}$  is the spatial time derivative of  $\psi$  at a fixed  $\mathbf{x}$ . Differentiate (2.84)<sub>2</sub> to obtain

$$\begin{aligned} \nabla \phi &= (\mathbf{F}^\pm)^T \text{grad } \psi, \quad \text{and} \\ \dot{\phi} &= \text{grad } \psi \cdot \mathbf{v}^\pm + \frac{\partial \psi}{\partial t}. \end{aligned} \quad (2.86)$$

The following relations can then be obtained on combining (2.49), (2.85) and (2.86):

$$\begin{aligned} \mathbf{n} &= \frac{(\mathbf{F}^\pm)^{-T} \mathbf{N}}{|(\mathbf{F}^\pm)^{-T} \mathbf{N}|}, \quad \text{and} \\ u &= \mathbf{n} \cdot \mathbf{v}^\pm + \frac{U}{|(\mathbf{F}^\pm)^{-T} \mathbf{N}|}. \end{aligned} \quad (2.87)$$

## 2.2 Balance laws and dissipation

Central to any theory of a continuous media are various integral theorems, which provide a mathematical framework for the interactions among various sub-bodies within the body and also for their interaction with the external environment. They also provide us means to express the global response of the body in terms of local relations. The theorems, stated (and proved) in the first subsection below, include localization theorems, divergence/Stokes' theorems, and transport theorems. In particular, we discuss them for fields which are piecewise smooth. In the next subsection we state the balance of mass, momentum and energy, first in an integral (global) form and then as differential equations away from the singular surface and jump conditions at the singular surface. The subsection is closed with a long remark on the interdependence of these balance laws. We end this section with the second law of thermodynamics. A brief motivation is first provided for taking Clausius-Duhem inequality as our starting point and then we go on to derive various consequences of this inequality pertinent to the discussion at hand.

### 2.2.1 Integral theorems

In this subsection we state and prove the localization theorem, the divergence theorem, the Stokes' theorem, and the transport theorem for volume and surface integrals. We have employed only elementary concepts from differential geometry in proving these theorems (see also the recent paper by Fosdick and Tang [53]). A more technical discussion can be accessed from the standard texts on differential geometry (for example, the book by Lee [104]).

**Localization theorem for volume integrals** Let  $\phi$  be a continuous function defined on an open set  $R \subset \mathcal{E}$ . If for all closed sets  $\pi \subset R$

$$\int_{\pi} \phi dV = 0, \quad (2.88)$$

then  $\phi(\mathbf{u}) = 0$  for all  $\mathbf{u} \in R$ . To prove this, we start by defining

$$I_{\varepsilon} = \left| \phi(\mathbf{u}_0) - \frac{1}{V_{\varepsilon}} \int_{s_{\varepsilon}} \phi(\mathbf{u}) dV \right| = \left| \frac{1}{V_{\varepsilon}} \int_{s_{\varepsilon}} (\phi(\mathbf{u}_0) - \phi(\mathbf{u})) dV \right|, \quad (2.89)$$

where  $s_{\varepsilon}$  is a sphere of radius  $\varepsilon$  and volume  $V_{\varepsilon}$  centered at  $\mathbf{u}_0 \in R$ . A theorem in analysis ([152], page 317) yields,

$$\begin{aligned} I_{\varepsilon} &\leq \frac{1}{V_{\varepsilon}} \int_{s_{\varepsilon}} |\phi(\mathbf{u}_0) - \phi(\mathbf{u})| dV \\ &\leq \frac{1}{V_{\varepsilon}} \int_{s_{\varepsilon}} \sup_{\mathbf{u} \in s_{\varepsilon}} |\phi(\mathbf{u}_0) - \phi(\mathbf{u})| dV \\ &= \max_{\mathbf{u} \in s_{\varepsilon}} |\phi(\mathbf{u}_0) - \phi(\mathbf{u})|, \end{aligned} \quad (2.90)$$

where in (2.90)<sub>2</sub>, sup can be replaced by max due to continuity and compactness of  $s_{\varepsilon}$ .

Since  $\phi(\mathbf{u})$  is continuous, we get  $I_{\varepsilon} \rightarrow 0$  as  $\varepsilon \rightarrow 0$ . It then follows from equation (2.89),

$$\phi(\mathbf{u}_0) = \lim_{\varepsilon \rightarrow 0} \frac{1}{V_{\varepsilon}} \int_{s_{\varepsilon}} \phi(\mathbf{u}) dV = 0, \quad (2.91)$$

where the last equality is a consequence of (2.88). The point  $\mathbf{u}_0$  can be chosen arbitrarily, and thus we can conclude that  $\phi(\mathbf{u}) = 0$  for all  $\mathbf{u} \in R$ .

**Localization theorem for surface integrals** Let  $\varphi$  be a continuous function defined on a surface  $\mathcal{F} \subset \mathcal{E}$ . If for all surfaces  $\zeta \subset \mathcal{F}$

$$\int_{\zeta} \varphi dA = 0, \quad (2.92)$$

then  $\varphi(\mathbf{u}) = 0$  for all  $\mathbf{u} \in \mathcal{F}$ . This can be proved using arguments similar to those used above.

**Divergence theorem for smooth fields** Let  $f$ ,  $\mathbf{p}$  and  $\mathbf{P}$  be respectively, scalar, vector and tensor fields defined on  $\kappa(\mathfrak{B}) \times (t_1, t_2)$ . Assume these fields to be continuously differentiable over  $\kappa(\mathfrak{B})$ . Then for any part  $\Omega \subset \kappa(\mathfrak{B})$  and at any time  $t \in (t_1, t_2)$

$$\int_{\Omega} (\nabla f) dV = \oint_{\partial\Omega} f \mathbf{N} dA, \quad (2.93)$$

$$\int_{\Omega} (\text{Div } \mathbf{p}) dV = \oint_{\partial\Omega} \mathbf{p} \cdot \mathbf{N} dA, \quad (2.94)$$

$$\int_{\Omega} (\text{Div } \mathbf{P}) dV = \oint_{\partial\Omega} \mathbf{P} \mathbf{N} dA, \quad (2.95)$$

where  $\mathbf{N} \in \mathcal{V}_{\kappa}$  is the outward unit normal to the boundary  $\partial\Omega$  of  $\Omega$ . For a proof of (2.94) see ([152], page 288). Equation (2.93) is obtained from (2.94) for a scalar  $\mathbf{p}$ . A proof for (2.95) also follows from (2.94). Indeed, for an arbitrary constant  $\mathbf{a} \in \mathcal{V}_{\kappa}$ ,

$$\mathbf{a} \cdot \oint_{\partial\Omega} \mathbf{P} \mathbf{N} dA = \oint_{\partial\Omega} (\mathbf{P}^T \mathbf{a}) \cdot \mathbf{N} dA = \int_{\Omega} (\text{Div } \mathbf{P}^T \mathbf{a}) dV = \int_{\Omega} (\text{Div } \mathbf{P}) \cdot \mathbf{a} dV, \quad (2.96)$$

where in the last equality, the definition of the Div operator has been used (cf. (2.19)).

Since  $\mathbf{a}$  is arbitrary, we get the desired result.

**Divergence theorem for piecewise smooth fields** Assume  $\mathbf{p}$  to be piecewise continuously differentiable over  $\kappa(\mathfrak{B})$ , being discontinuous across the singular surface  $S_t$  (with normal  $\mathbf{N}_s$  and speed  $U$ ) and smooth everywhere else. Then for a domain  $\Omega$  such that  $\mathcal{S} = \Omega \cap S_t \neq \emptyset$ ,

$$\oint_{\partial\Omega} \mathbf{p} \cdot \mathbf{N} dA = \int_{\Omega} (\text{Div } \mathbf{p}) dV + \int_{\mathcal{S}} [[\mathbf{p}]] \cdot \mathbf{N}_s dA. \quad (2.97)$$

Similar statements hold for scalar and tensor fields. We now prove (2.97). Let  $\Omega^{\pm} \subset \Omega$  be such that  $\Omega^+ \cup \Omega^- = \Omega$  and  $\Omega^+ \cap \Omega^- = \mathcal{S}$ . The normal to the surface  $\mathcal{S}$  is oriented such

that it points into  $\Omega^+$ . Since  $\mathbf{p}$  is smooth within  $\Omega^+$  and  $\Omega^-$ , we can use (2.94) to write

$$\begin{aligned}\int_{\Omega^+} (\text{Div } \mathbf{p}) dV &= \int_{\partial\Omega^+ \setminus \mathcal{S}} \mathbf{p} \cdot \mathbf{N} dA - \int_{\mathcal{S}} \mathbf{p}^+ \cdot \mathbf{N}_s dA, \\ \int_{\Omega^-} (\text{Div } \mathbf{p}) dV &= \int_{\partial\Omega^- \setminus \mathcal{S}} \mathbf{p} \cdot \mathbf{N} dA + \int_{\mathcal{S}} \mathbf{p}^- \cdot \mathbf{N}_s dA,\end{aligned}$$

where  $\mathbf{p}^\pm$  are the limiting values of  $\mathbf{p}$  as it approaches  $\mathcal{S}$  from the interior of  $\Omega^\pm$ . The relation (2.97) is obtained by adding these two equations.

If  $\mathbf{q}$  is a vector field defined on  $\chi(\mathfrak{B}) \times (t_1, t_2)$  and piecewise continuously differentiable over  $\chi(\mathfrak{B})$ , being discontinuous across the singular surface  $s_t$  (with normal  $\mathbf{n}_s$  and speed  $u$ ). Then for  $\omega \subset \chi(\mathfrak{B})$  such that  $s = \omega \cap s_t \neq \emptyset$ ,

$$\oint_{\partial\omega} \mathbf{q} \cdot \mathbf{n} da = \int_{\omega} (\text{div } \mathbf{q}) dv + \int_s [[\mathbf{q}]] \cdot \mathbf{n}_s da. \quad (2.98)$$

The proof for (2.98) is similar to that of (2.97).

**Stokes' theorem for smooth fields** Let  $\mathbf{p}$  and  $\mathbf{P}$  be respectively, vector and tensor fields defined on  $\kappa(\mathfrak{B}) \times (t_1, t_2)$ . Assume these fields to be continuously differentiable over  $\kappa(\mathfrak{B})$ . Then for any surface  $\mathcal{F} \subset \kappa(\mathfrak{B})$  with normal  $\mathbf{N}$  and boundary  $\partial\mathcal{F}$

$$\int_{\mathcal{F}} (\text{Curl } \mathbf{p}) \cdot \mathbf{N} dA = \oint_{\partial\mathcal{F}} \mathbf{p} \cdot d\mathbf{X}, \quad (2.99)$$

$$\int_{\mathcal{F}} (\text{Curl } \mathbf{P})^T \mathbf{N} dA = \oint_{\partial\mathcal{F}} \mathbf{P} d\mathbf{X}. \quad (2.100)$$

A proof for (2.99) can be obtained from ([152], page 287). To verify (2.100), we use (2.99).

Indeed, for an arbitrary constant vector  $\mathbf{a} \in \mathcal{V}_\kappa$ ,

$$\mathbf{a} \cdot \int_{\mathcal{F}} (\text{Curl } \mathbf{P})^T \mathbf{N} dA = \int_{\mathcal{F}} (\text{Curl } \mathbf{P}^T \mathbf{a}) \cdot \mathbf{N} dA = \mathbf{a} \cdot \oint_{\partial\mathcal{F}} \mathbf{P} d\mathbf{X}, \quad (2.101)$$

where in the first equality, the definition of the Curl of a tensor field (cf. (2.20)) is used.

The desired result follows upon using the arbitrariness of  $\mathbf{a}$ .

**Stokes' theorem for piecewise smooth fields** Consider  $\mathbf{p}$  to be piecewise continuously differentiable over  $\kappa(\mathfrak{B})$ . Assume  $\mathbf{p}$  to be discontinuous across the singular surface  $S_t$  and smooth everywhere else. Let  $\Gamma = \mathcal{F} \cap S_t$  be the curve of intersection. Then

$$\int_{\mathcal{F}} (\text{Curl } \mathbf{p}) \cdot \mathbf{N} dA = \oint_{\partial \mathcal{F}} \mathbf{p} \cdot d\mathbf{X} + \int_{\Gamma} [[\mathbf{p}]] \cdot d\mathbf{X}. \quad (2.102)$$

To verify this relation start by considering two subsurfaces  $\mathcal{F}^{\pm} \subset \mathcal{F}$  such that  $\mathcal{F}^+ \cup \mathcal{F}^- = \mathcal{F}$  and  $\mathcal{F}^+ \cap \mathcal{F}^- = \Gamma$ . Since  $\mathbf{p}$  is smooth in regions  $\mathcal{F}^{\pm}$ , we can write using (2.99)

$$\begin{aligned} \int_{\mathcal{F}^+} (\text{Curl } \mathbf{p}) \cdot \mathbf{N} dA &= \int_{\partial \mathcal{F}^+ \setminus \Gamma} \mathbf{p} \cdot d\mathbf{X} + \int_{\Gamma} \mathbf{p}^+ \cdot d\mathbf{X}, \\ \int_{\mathcal{F}^-} (\text{Curl } \mathbf{p}) \cdot \mathbf{N} dA &= \int_{\partial \mathcal{F}^- \setminus \Gamma} \mathbf{p} \cdot d\mathbf{X} - \int_{\Gamma} \mathbf{p}^- \cdot d\mathbf{X}. \end{aligned}$$

Adding these two relations we get (2.102). Similarly, we obtain for a piecewise continuously differentiable tensor field  $\mathbf{P}$ :

$$\int_{\mathcal{F}} (\text{Curl } \mathbf{P})^T \mathbf{N} dA = \oint_{\partial \mathcal{F}} \mathbf{P} d\mathbf{X} + \int_{\Gamma} [[\mathbf{P}]] d\mathbf{X}. \quad (2.103)$$

If  $\mathbf{q}$  is a piecewise continuously differentiable vector field defined on  $\chi(\mathfrak{B}) \times (t_1, t_2)$ , being discontinuous across the singular surface  $s_t$ . Consider a surface  $F \subset \chi(\mathfrak{B})$  with normal  $\mathbf{n}$  and let  $\gamma = F \cap s_t$ . Then

$$\int_F (\text{curl } \mathbf{q}) \cdot \mathbf{n} da = \oint_{\partial F} \mathbf{q} \cdot d\mathbf{x} + \int_{\gamma} [[\mathbf{q}]] \cdot d\mathbf{x}. \quad (2.104)$$

The proof for (2.104) is similar to that of (2.102).

*Remark 2.2.1.* (Surface divergence theorem) Consider a vector field  $\mathbf{p}$  continuously differentiable over the surface  $S \subset \kappa(\mathfrak{B})$  (with unit normal  $\mathbf{N}$  and mean curvature  $H$ ) for a fixed time interval  $(t_1, t_2)$ . Then

$$\oint_{\partial S} \mathbf{p} \cdot \boldsymbol{\nu} dL = \int_S (\text{Div}^S \mathbf{p} + 2H\mathbf{p} \cdot \mathbf{N}) dA, \quad (2.105)$$

where  $\boldsymbol{\nu}$  is the outer unit normal to  $\partial S$  such that  $(\mathbf{N}, \boldsymbol{\nu}, \mathbf{t})$  form a positively-oriented orthogonal triad at  $\partial S$  with  $\mathbf{t}$  being the tangent vector along  $\partial S$ . Moreover, if  $\mathbf{p}$  is tangential, i.e.  $\mathbb{P}\mathbf{p} = \mathbf{p}$ , then  $\mathbf{p} \cdot \mathbf{N} = 0$  and (2.105) reduces to

$$\oint_{\partial S} \mathbf{p} \cdot \boldsymbol{\nu} dL = \int_S \text{Div}^S \mathbf{p} dA. \quad (2.106)$$

We now prove (2.105). By definition  $\boldsymbol{\nu} = \mathbf{t} \times \mathbf{N}$  and therefore we can use Stokes' theorem to rewrite the term on the left hand side of equation (2.105) as

$$\begin{aligned} \oint_{\partial S} \mathbf{p} \cdot \boldsymbol{\nu} dL &= \oint_{\partial S} \mathbf{p} \cdot (\mathbf{t} \times \mathbf{N}) dL \\ &= \oint_{\partial S} (\mathbf{N} \times \mathbf{p}) \cdot \mathbf{t} dL \\ &= \int_S \text{Curl}(\mathbf{N} \times \mathbf{p}) \cdot \mathbf{N} dA. \end{aligned} \quad (2.107)$$

Use the identity  $\text{Curl}(\mathbf{N} \times \mathbf{p}) = \text{Div}(\mathbf{N} \otimes \mathbf{p} - \mathbf{p} \otimes \mathbf{N})$  to get

$$\text{Curl}(\mathbf{N} \times \mathbf{p}) \cdot \mathbf{N} = (\nabla \mathbf{N})^T \mathbf{N} \cdot \mathbf{p} - (\mathbf{p} \cdot \mathbf{N}) \text{Div} \mathbf{N} + \nabla \mathbf{p} \cdot \mathbb{P}. \quad (2.108)$$

But  $(\nabla \mathbf{N})^T \mathbf{N} = \mathbf{0}$  (follows from  $\mathbf{N} \cdot \mathbf{N} = 1$ ) and  $\nabla \mathbf{p} \cdot \mathbb{P} = \text{tr}(\nabla \mathbf{p} \mathbb{P}) = \text{Div}^S \mathbf{p}$ . Furthermore, it follows from (2.57) and (2.58) that  $\text{Div} \mathbf{N} = -2H$ . Therefore we can rewrite (2.108) to get

$$\text{Curl}(\mathbf{N} \times \mathbf{p}) \cdot \mathbf{N} = 2H(\mathbf{p} \cdot \mathbf{N}) + \text{Div}^S \mathbf{p}. \quad (2.109)$$

Substituting this into (2.107) yields (2.105).

**Transport theorem for volume integrals with smooth fields** Let  $P$  and  $Q$  denote a scalar, vector or tensor field continuously differentiable on  $\kappa(\mathfrak{B}) \times (t_1, t_2)$  and  $\chi(\mathfrak{B}) \times (t_1, t_2)$ ,



respectively. Then for arbitrary parts  $\Omega \subset \kappa(\mathfrak{B})$ ,  $\omega \subset \chi(\mathfrak{B})$  and at any time  $t \in (t_1, t_2)$

$$\frac{d}{dt} \int_{\Omega} P dV = \int_{\Omega} \dot{P} dV, \quad (2.110)$$

$$\frac{d}{dt} \int_{\omega} Q dv = \int_{\omega} \frac{\partial Q}{\partial t} dv + \int_{\partial\omega} Q(\mathbf{v} \cdot \mathbf{n}) da. \quad (2.111)$$

Since  $\Omega$  is fixed with respect to time and  $P$  is smooth over  $\Omega$ , the time derivative and the volume integral in the left hand side of (2.110) can commute to give the right hand side of the equation. Equation (2.111) can be proved by first transforming the volume  $\omega$  to a fixed reference volume, say  $\Omega$ . We get

$$\begin{aligned} \frac{d}{dt} \int_{\omega} Q dv &= \frac{d}{dt} \int_{\Omega} Q J dV \\ &= \int_{\Omega} \dot{Q} dv + \int_{\Omega} Q(\operatorname{div} \mathbf{v}) dv, \end{aligned} \quad (2.112)$$

where  $J$  is the jacobian associated with the mapping which transforms  $\Omega$  to  $\omega$  and  $\dot{J} = J(\operatorname{div} \mathbf{v})$ . Equation (2.111) follows from (2.112) upon recalling the definition of the material time derivative (cf. (2.9)) and using the divergence theorem.

**Transport theorem for volume integrals with piecewise smooth fields** Let  $\Omega$  be such that  $\mathcal{S} = \Omega \cap S_t \neq \emptyset$ . Then for a  $P$  which is discontinuous across  $S_t$  but smooth everywhere else,

$$\frac{d}{dt} \int_{\Omega} P dV = \int_{\Omega} \dot{P} dV - \int_{\mathcal{S}} U[[P]] dA. \quad (2.113)$$

We now prove this relation. Recall surface parametrization from the end of subsection 2.1.4. In a small neighborhood, say  $\Omega_{\mathcal{S}}$ , of the singular surface  $\mathcal{S}$  we parameterize the domain by coordinates  $\{\xi_1, \xi_2, \zeta\}$  such that for  $\mathbf{X} \in \Omega_{\mathcal{S}}$  we can write  $\mathbf{X} = \hat{\mathbf{X}}(\xi_1, \xi_2, t) + \zeta(t)\mathbf{N}(\xi_1, \xi_2, t)$ , where  $\hat{\mathbf{X}} \in \mathcal{S}$  and  $\{\xi_1, \xi_2\}$  are convected. Let  $-\varsigma < \zeta(t) < \varsigma$ , where  $\varsigma \in \mathbb{R}^+$  is constant. The

position of the singular surface is indicated by  $\zeta = 0$  and it is assumed that the surface  $\mathcal{S}$  remains inside  $\Omega_{\mathcal{S}}$  during the instantaneous motion. Obtain

$$\begin{aligned} \frac{d}{dt} \int_{\Omega} P dV &= \frac{d}{dt} \int_{\Omega \setminus \Omega_{\mathcal{S}}} P dV + \frac{d}{dt} \int_{\Omega_{\mathcal{S}}} P dV \\ &= \int_{\Omega \setminus \Omega_{\mathcal{S}}} \dot{P} dV + \int_{(\xi_1, \xi_2)} \frac{d}{dt} \left( \int_{-\zeta}^{\zeta} P j_A d\zeta \right) dA_{\xi}, \\ &= \int_{\Omega \setminus \Omega_{\mathcal{S}}} \dot{P} dV + \int_{(\xi_1, \xi_2)} \left\{ \frac{d}{dt} \left( \int_{-\zeta}^{\zeta_1(t)} P j_A d\zeta + \int_{\zeta_2(t)}^{\zeta} P j_A d\zeta \right) \right\}_{\zeta_1, \zeta_2=0} dA_{\xi}, \end{aligned}$$

where  $j_A$  is the jacobian related to the change of coordinates. On the singular surface,  $\zeta_1 = \zeta_2 = 0$ ,  $\dot{\zeta}_1 = \dot{\zeta}_2 = U$ ,  $j_A = \xi$  (cf. (2.81)) and  $dA = \xi dA_{\xi}$ , where  $\xi$  is the surface jacobian. Taking the limit  $|\zeta| \rightarrow 0$  we obtain the desired result. The infinitesimal area of the surface in terms of the new coordinates can be obtained by using Nanson's formula,  $\mathbf{N} dA = j_A \mathbf{A}^{-T} \hat{\mathbf{N}} dA_{\xi}$ , where  $\hat{\mathbf{N}} = \mathbf{N}$  and  $\mathbf{A}$  is the gradient of the map from the new coordinates to  $\mathbf{X}$ . For the considered transformation this formula reduces to  $dA = j_A dA_{\xi}$  (cf. (2.80)).

Let  $\omega$  be such that  $s = \omega \cap s_t \neq \emptyset$ . Then for a  $Q$  which is discontinuous across  $s_t$  but smooth everywhere else,

$$\frac{d}{dt} \int_{\omega} Q dv = \int_{\omega} \left( \frac{\partial Q}{\partial t} + \text{div}(Q \mathbf{v}) \right) dv - \int_s (u \llbracket Q \rrbracket - \llbracket Q \mathbf{v} \rrbracket \cdot \mathbf{n}) da, \quad (2.114)$$

where  $u = U |(\mathbf{F}^{\pm})^T \mathbf{n}| + \mathbf{n} \cdot \mathbf{v}^{\pm}$  is the spatial speed of the singular surface  $s_t$ . This relation can be proved by first transforming  $\omega$  to  $\Omega$  and then using (2.113). We get

$$\frac{d}{dt} \int_{\omega} Q dv = \int_{\Omega} (JQ) dV - \int_S U \llbracket JQ \rrbracket dA. \quad (2.115)$$

The term  $U \llbracket JQ \rrbracket$  can be expanded as

$$\begin{aligned} U \llbracket JQ \rrbracket &= (Q^+ u^+ J^+ |(\mathbf{F}^+)^{-T} \mathbf{N}|) - (Q^- u^- J^- |(\mathbf{F}^-)^{-T} \mathbf{N}|) \\ &= (u \llbracket Q \rrbracket - \llbracket Q \mathbf{v} \rrbracket \cdot \mathbf{n}) |(\mathbf{F}^-)^* \mathbf{N}|, \end{aligned} \quad (2.116)$$

where  $u^\pm = u - \mathbf{n} \cdot \mathbf{v}^\pm$ . Relations  $U = u^\pm |(\mathbf{F}^\pm)^{-T} \mathbf{N}|$  and  $|(\mathbf{F}^+)^* \mathbf{N}| = |(\mathbf{F}^-)^* \mathbf{N}|$  have also been used. Equation (2.114) follows immediately after substituting (2.116) into (2.115).

**Transport theorem for surface integrals with smooth fields** Let  $p$  be a scalar, vector or tensor field continuously differentiable on  $S_t \times (t_1, t_2)$ . Then, for an arbitrary surface  $\mathcal{S} \subset S_t$

$$\frac{d}{dt} \int_{\mathcal{S}} p dA = \int_{\mathcal{S}} (\dot{p} - 2pUH) dA, \quad (2.117)$$

where  $\mathbf{N}$ ,  $U$ , and  $H$  are the unit normal, normal velocity, and the mean curvature associated with  $S_t$ , respectively. We prove this relation using the surface parametrization outlined in subsection 2.1.4. We assume that  $p$  can be extended to the small neighborhood  $\Omega_{\mathcal{S}}$ , and use the same symbol to denote its extension. Obtain

$$\begin{aligned} \frac{d}{dt} \int_{\mathcal{S}} p dA &= \left\{ \frac{d}{dt} \int_{(\xi_1, \xi_2)} p(\mathbf{X}(\xi_\alpha, \zeta(t)), t) j_A dA_\xi \right\}_{\zeta=0} \\ &= \int_{(\xi_1, \xi_2)} \{ (\dot{p} j_A + j_A \dot{\zeta} (\nabla p \cdot \mathbf{N}) + p \dot{j}_A) dA_\xi \}_{\zeta=0} \\ &= \int_{\mathcal{S}} \{ \dot{p} + \dot{\zeta} \nabla p \cdot \mathbf{N} + p \dot{j}_A j_A^{-1} \}_{\zeta=0} dA. \end{aligned} \quad (2.118)$$

At the surface,  $\zeta = 0$ , we have  $\dot{\zeta} = U$ ,  $j_A = \xi$  and  $\dot{j}_A = -2UH\xi$  (cf. (2.81)). Substituting these into (2.118) and recalling the definition of the normal time derivative from (2.60), we obtain (2.117).

### 2.2.2 Balance laws and jump conditions

Let  $\mathbf{p}$ ,  $\mathbf{r}$  and  $\mathbf{s}$  be piecewise continuously differentiable vector fields on  $\kappa(\mathfrak{B}) \times (t_1, t_2)$ . A global (or integral) *balance law* is a relation of the following form: For an

arbitrary  $\Omega \subset \kappa(\mathfrak{B})$ ,

$$\frac{d}{dt} \int_{\Omega} \mathbf{p} dV = \int_{\Omega} \mathbf{r} dV + \int_{\partial\Omega} \mathbf{s} dA. \quad (2.119)$$

This relation expresses the integral form of the balance of the change in the quantity  $\mathbf{p}$  with a volume supply/sink density  $\mathbf{r}$  and a surface interaction  $\mathbf{s}$ .

**Surface interactions** Given that a balance law of the form (2.119) exists, the surface interaction vector  $\mathbf{s}$  depends on the surface only through the unit normal and moreover the dependence is linear. The first claim was introduced by Cauchy in 1823 (for an historical account see footnotes in [171], sections 200 & 203) as a hypothesis and was proved much later in 1959 by Noll [131]. The second claim, which is also known as the Cauchy's theorem, is based on the classical tetrahedron argument first proposed by Cauchy and is now recognized as a result of fundamental importance in continuum physics. These classical derivations are restricted to continuously differentiable fields defined on domains with piecewise smooth boundaries. Much research has been done in the past fifty years to investigate these results under less stringent smoothness requirements. Such considerations are indeed necessary for many practical problems in mechanics such as those involving shocks, fracture, dislocations and corner singularities (for a recent contribution, where most of the past work is carefully reviewed, see [153]). In the following we state the theorems of Noll and Cauchy, whose proofs are available in most of the standard texts on continuum mechanics.

According to *Cauchy's hypothesis (Noll's theorem)*, if  $\mathbf{N}$  is the outward unity normal to the positively oriented surface  $\partial\Omega$ , then

$$\mathbf{s}(\mathbf{X}, t; \partial\Omega) = \mathbf{s}(\mathbf{X}, t; \mathbf{N}), \quad (2.120)$$

i.e. the dependence of the surface interaction vector on the surface on which it acts is only through the normal  $\mathbf{N}$ . According to *Cauchy's theorem*, the surface interaction vector  $\mathbf{s}$  depends linearly on  $\mathbf{N}$ . Therefore, there exists a tensor  $\mathbf{S}$  such that

$$\mathbf{s}(\mathbf{X}, t; \mathbf{N}) = \mathbf{S}(\mathbf{X}, t)\mathbf{N}. \quad (2.121)$$

We now obtain local statements of the fundamental balance laws in continuum mechanics. The fields are allowed to be piecewise continuously differentiable so that they may suffer jump discontinuities across a surface in the domain over which they are defined. Consider an arbitrary part of the body,  $\mathfrak{S} \subset \mathfrak{B}$ , whose placement in the reference and current configurations is denoted by  $\Omega = \kappa(\mathfrak{S})$  and  $\omega = \chi(\mathfrak{S})$ , respectively. Let  $\mathcal{S} = \Omega \cap S_t$ , where  $S_t$  is the singular surface in  $\kappa(\mathfrak{B})$  with normal  $\mathbf{N}_s$  and speed  $U$ . Correspondingly let  $s = \omega \cap s_t$ , where  $s_t$  is the singular surface in  $\chi(\mathfrak{B})$  with normal  $\mathbf{n}_s$  and speed  $u$ .

*Remark 2.2.2.* Here we have made an implicit assumption regarding the coherency of the interface, i.e.  $[[\chi_\kappa]] = \mathbf{0}$ . In the absence of coherency, the referential interface  $S_t$  will be mapped into two distinct surfaces in the current configuration, rather than an interface  $s_t$ . In case of an incoherent interface, global balance laws are written only in the reference configuration (since the spatial configuration is disconnected). The local balance laws in the spatial configuration can be obtained from the local balance laws in the reference configuration using appropriate transformations. In the following we will, however, restrict our attention to coherent interfaces (see [29] for a detailed account on incoherent interfaces).

**Balance of mass** Define a *mass* function  $m \in \mathbb{R}$  such that:

$$(i) \quad m(\mathfrak{S}) \geq 0, \quad \forall \mathfrak{S} \subset \mathfrak{B},$$

(ii)  $m(\emptyset) = 0$  and

(iii) Let  $\{\mathfrak{S}_i\}_{i=1}^{\infty}$  be a disjoint family of subsets of the body  $\mathfrak{B}$ , i.e.  $\mathfrak{S}_i \cap \mathfrak{S}_j = \emptyset$ ,  $i \neq j$ .

Then  $m(\bigcup_{i=1}^{\infty} \mathfrak{S}_i) = \sum_{i=1}^{\infty} m(\mathfrak{S}_i)$ .

Therefore the function  $m$  is a measure on  $\mathfrak{B}$ . Denote by  $V$  and  $v$  respectively, the volume of  $\mathfrak{S}$  in the reference configuration and the current configuration. Define the density of mass in the reference and the current configuration by

$$0 < \rho_{\kappa}(\mathbf{X}, t) = \lim_{V \rightarrow 0} \frac{m(\mathfrak{S}, t)}{V} \quad (2.122)$$

and

$$0 < \rho(\mathbf{x}, t) = \lim_{v \rightarrow 0} \frac{m(\mathfrak{S}, t)}{v}, \quad (2.123)$$

respectively, where  $\mathbf{X} \in \Omega$  and  $\mathbf{x} \in \omega$ . The existence of limits is assumed in the above definitions. The mass of the part  $\mathfrak{S} \subset \mathfrak{B}$  is then given by

$$m(\mathfrak{S}, t) = \int_{\Omega} \rho_{\kappa}(\mathbf{X}, t) dV = \int_{\omega} \rho(\mathbf{x}, t) dv. \quad (2.124)$$

The reference mass density can be related to the current density of mass by using the jacobian  $J_F = \det \mathbf{F} > 0$ , such that  $J_F dV = dv$  (and  $d\mathbf{x} = \mathbf{F}d\mathbf{X}$ ), and the localization theorem in (2.124). We get

$$\rho_{\kappa} = J_F \rho. \quad (2.125)$$

Assuming (for now) an absence of diffusion and any external source of mass, we express the law of balance of mass as

$$\dot{m}(\mathfrak{S}, t) = 0 \quad (2.126)$$

or from (2.124)

$$\frac{d}{dt} \int_{\Omega} \rho_{\kappa}(\mathbf{x}, t) dv = 0, \quad (2.127)$$

which, on using the transport theorem (2.113), reduces to

$$\int_{\Omega} \dot{\rho}_{\kappa} dV - \int_{\mathcal{S}} U[[\rho_{\kappa}]] dA = 0. \quad (2.128)$$

We can choose  $\Omega$  such that  $\mathcal{S} = \emptyset$ . Thereupon using the localization theorem we obtain

$$\dot{\rho}_{\kappa} = 0 \quad (2.129)$$

outside the singular surface. The referential mass density is therefore independent of time.

For  $\mathcal{S} \neq \emptyset$ , substitution of (2.129) in (2.128) reduces it to a surface integral. Using the arbitrariness of  $\mathcal{S}$ , the localization theorem for surface integrals then yields the following jump condition at the singular surface

$$U[[\rho_{\kappa}]] = 0, \quad (2.130)$$

i.e. either the normal speed vanishes or the referential mass density is continuous across  $S_t$ .

The spatial form of the balance law reads

$$\frac{d}{dt} \int_{\omega} \rho(\mathbf{x}, t) dv = 0, \quad (2.131)$$

which, on using the transport theorem (2.114) and the localization theorem, yields

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \mathbf{v}) = 0 \quad (2.132)$$

outside the singular surface and

$$(u[[\rho]] - [[\rho \mathbf{v}]] \cdot \mathbf{n}_s) = 0 \quad (2.133)$$

on the singular surface  $s_t$ .

**Balance of linear and angular momentum** We assume that the forces acting on  $\mathfrak{S}$  are either contact forces or body forces. A *contact force* arises from the contact of two parts of  $\mathfrak{B}$ , say  $\mathfrak{S}_1$  and  $\mathfrak{S}_2$ . The force exerted by  $\mathfrak{S}_2$  on  $\mathfrak{S}_1$  is given by

$$\mathbf{F}_c(\mathfrak{S}_1, \mathfrak{S}_2, t) = \int_I \mathbf{p} dA = \int_i \mathbf{t} da, \quad (2.134)$$

where  $I = \kappa(\mathfrak{S}_1) \cap \kappa(\mathfrak{S}_2)$  and  $i = \chi(\mathfrak{S}_1) \cap \chi(\mathfrak{S}_2)$ . The vector  $\mathbf{p}$  is the contact force per unit area of  $\partial\Omega$  (Piola traction force) and  $\mathbf{t}$  is the contact force per unit area of  $\partial\omega$  (Cauchy traction force). A *body force* arises from the interaction of  $\mathfrak{S}$  with sources external to  $\mathfrak{S}$  (e.g. gravitational force). It can be of two kinds: one due to effects exterior to  $\mathfrak{B}$  and the other due to effects due to the matter in  $\mathfrak{B} \setminus \mathfrak{S}$ . It acts on the particles comprising the body and has a form

$$\mathbf{F}_b(\mathfrak{S}, t) = \int_{\Omega} \rho_{\kappa} \mathbf{b} dV = \int_{\omega} \rho \mathbf{b} dv, \quad (2.135)$$

where  $\mathbf{b} = \hat{\mathbf{b}}(\mathbf{X}, t) = \tilde{\mathbf{b}}(\mathbf{x}, t)$  is the body force per unit mass. The total force on  $\mathfrak{S}$  can then be written as

$$\mathbf{F}(\mathfrak{S}, t) = \mathbf{F}_c(\mathfrak{S}, \mathfrak{B} \setminus \mathfrak{S}, t) + \mathbf{F}_b(\mathfrak{S}, t). \quad (2.136)$$

Associated with these forces are *moments*. The moments of the contact force and the body force with respect to an arbitrary point  $\mathbf{x}_0 \in \mathcal{E}$  are respectively,

$$\begin{aligned} \mathbf{M}_c(\mathfrak{S}_1, \mathfrak{S}_2, t; \mathbf{x}_0) &= \int_I (\mathbf{x} - \mathbf{x}_0) \times \mathbf{p} dA = \int_i (\mathbf{x} - \mathbf{x}_0) \times \mathbf{t} da, \text{ and} \\ \mathbf{M}_b(\mathfrak{S}, t; \mathbf{x}_0) &= \int_{\Omega} \rho_{\kappa} (\mathbf{x} - \mathbf{x}_0) \times \mathbf{b} dV = \int_{\omega} \rho (\mathbf{x} - \mathbf{x}_0) \times \mathbf{b} dv. \end{aligned} \quad (2.137)$$

The total moment acting upon  $\mathfrak{S}$  is

$$\mathbf{M}(\mathfrak{S}, t; \mathbf{x}_0) = \mathbf{M}_c(\mathfrak{S}, \mathfrak{B} \setminus \mathfrak{S}, t; \mathbf{x}_0) + \mathbf{M}_b(\mathfrak{S}, t; \mathbf{x}_0). \quad (2.138)$$



The linear momentum of  $\mathfrak{S} \subset \mathfrak{B}$  is given by

$$\mathbf{G}(\mathfrak{S}, t) = \int_{\Omega} \rho_{\kappa} \mathbf{v} dV = \int_{\omega} \rho \mathbf{v} dv. \quad (2.139)$$

The balance of linear momentum can be stated in the form of Euler's first postulate of motion: The rate of change of linear momentum of  $\mathfrak{S}$  is equal to the total force acting on  $\mathfrak{S}$ , i.e.

$$\dot{\mathbf{G}}(\mathfrak{S}, t) = \mathbf{F}(\mathfrak{S}, t). \quad (2.140)$$

The referential (or material) form of the balance of linear momentum obtained by substituting definitions (2.136) and (2.139) into (2.140) is

$$\frac{d}{dt} \int_{\Omega} \rho_{\kappa} \mathbf{v} dV = \int_{\partial\Omega} \mathbf{p} dA + \int_{\Omega} \rho_{\kappa} \mathbf{b} dV. \quad (2.141)$$

By Noll's and Cauchy's theorems there exists a tensor field  $\mathbf{P}$  such that  $\mathbf{p} = \mathbf{P}\mathbf{N}$ . The tensor  $\mathbf{P}$  is called the Piola-Kirchhoff stress tensor. Use the transport theorem (2.113) and the divergence theorem (2.97) to get

$$\int_{\Omega} \rho_{\kappa} \dot{\mathbf{v}} dV - \int_{\mathcal{S}} U \rho_{\kappa} [[\mathbf{v}]] dA = \int_{\Omega} \text{Div } \mathbf{P} dV + \int_{\mathcal{S}} [[\mathbf{P}]] \mathbf{N}_s + \int_{\Omega} \rho_{\kappa} \mathbf{b} dV, \quad (2.142)$$

where we have also used (2.129) and (2.130). Since  $\Omega$  is arbitrary, we can choose it such that  $\mathcal{S} = \emptyset$ . The localization theorem then yields the local form for the balance of linear momentum

$$\rho_{\kappa} \dot{\mathbf{v}} = \text{Div } \mathbf{P} + \rho_{\kappa} \mathbf{b}, \quad (2.143)$$

which holds outside the singular surface. Now consider  $\mathcal{S} \neq \emptyset$ . Substitute (2.143) in (2.142) and use the arbitrariness of  $\mathcal{S}$  to use the localization theorem to obtain the jump condition across  $S_t$

$$U \rho_{\kappa} [[\mathbf{v}]] + [[\mathbf{P}]] \mathbf{N}_s = \mathbf{0}. \quad (2.144)$$

The spatial form of these equations can be obtained in a similar manner. We write the spatial form of the balance of linear momentum as

$$\frac{d}{dt} \int_{\omega} \rho \mathbf{v} dv = \int_{\partial\omega} \mathbf{t} dA + \int_{\omega} \rho \mathbf{b} dv. \quad (2.145)$$

By Noll's and Cauchy's theorems there exists a tensor field  $\mathbf{T}$  such that  $\mathbf{t} = \mathbf{T}\mathbf{n}$ . The tensor  $\mathbf{T}$  is called the Cauchy stress tensor. The local form of the balance law can be now obtained using the transport theorem (2.114), the divergence theorem (2.98) and the localization theorem. We obtain outside the singular surface and on the singular surface respectively,

$$\rho \dot{\mathbf{v}} = \operatorname{div} \mathbf{T} + \rho \mathbf{b} \quad (2.146)$$

and

$$j_s \llbracket \mathbf{v} \rrbracket + \llbracket \mathbf{T} \rrbracket \mathbf{n}_s = \mathbf{0}, \quad (2.147)$$

where

$$j_s = \frac{\rho_{\kappa} U}{|(\mathbf{F}^{\pm})^* \mathbf{N}_s|}$$

is the flux of mass through the singular surface. Use (2.87)<sub>2</sub> to rewrite (2.147) as

$$\rho^{\pm} (u - \mathbf{n}_s \cdot \mathbf{v}^{\pm}) \llbracket \mathbf{v} \rrbracket + \llbracket \mathbf{T} \rrbracket \mathbf{n}_s = \mathbf{0}. \quad (2.148)$$

The moment of momentum of  $\mathfrak{S} \subset \mathfrak{B}$  relative to an arbitrary  $\mathbf{x}_0 \in \mathcal{E}$  is given by

$$\mathbf{H}(\mathfrak{S}, t; \mathbf{x}_0) = \int_{\Omega} \rho_{\kappa} (\mathbf{x} - \mathbf{x}_0) \times \mathbf{v} dV = \int_{\omega} \rho (\mathbf{x} - \mathbf{x}_0) \times \mathbf{v} dv. \quad (2.149)$$

The balance of angular momentum in the form of Euler's second postulate of motion is the following: The rate of change of moment of momentum of  $\mathfrak{S}$  is equal to the total moment acting on  $\mathfrak{S}$ , i.e.

$$\dot{\mathbf{H}}(\mathfrak{S}, t; \mathbf{x}_0) = \mathbf{M}(\mathfrak{S}, t; \mathbf{x}_0). \quad (2.150)$$

Substituting equations (2.138) and (2.149) into (2.150) we get the referential form of the balance of angular momentum

$$\frac{d}{dt} \int_{\Omega} \rho_{\kappa}(\mathbf{x} - \mathbf{x}_0) \times \mathbf{v} dV = \int_{\partial\Omega} (\mathbf{x} - \mathbf{x}_0) \times \mathbf{p} dA + \int_{\Omega} \rho_{\kappa}(\mathbf{x} - \mathbf{x}_0) \times \mathbf{b} dV. \quad (2.151)$$

The local form outside the singular surface is

$$\rho_{\kappa}((\mathbf{x} - \mathbf{x}_0) \times \mathbf{v})' = \text{Div}((\mathbf{x} - \mathbf{x}_0) \times \mathbf{P}) + \rho_{\kappa}(\mathbf{x} - \mathbf{x}_0) \times \mathbf{b}, \quad (2.152)$$

where for any  $\mathbf{y} \in \mathcal{V}$ ,  $(\mathbf{y} \times \mathbf{P})_{il} = e_{ijk} y_j P_{kl}$ . On using (2.143), (2.152) leads to

$$\mathbf{P}\mathbf{F}^T = \mathbf{F}\mathbf{P}^T. \quad (2.153)$$

The jump condition is

$$U\rho_{\kappa}[[\mathbf{x} - \mathbf{x}_0) \times \mathbf{v}] + [(\mathbf{x} - \mathbf{x}_0) \times \mathbf{P}\mathbf{N}_s] = \mathbf{0}, \quad (2.154)$$

which can be rewritten using (2.46) as

$$\langle \mathbf{x} - \mathbf{x}_0 \rangle \times (U\rho_{\kappa}[[\mathbf{v}] + [[\mathbf{P}]]\mathbf{N}_s) + [[\mathbf{x}]] \times (U\rho_{\kappa}\langle \mathbf{v} \rangle + \langle \mathbf{P} \rangle \mathbf{N}_s) = \mathbf{0}. \quad (2.155)$$

Jump conditions (2.130) and (2.144) imply that the term  $(U\rho_{\kappa}\mathbf{v} + \mathbf{P}\mathbf{N}_s)$  is continuous across  $\mathcal{S}$ , thereby reducing (2.155) to

$$[[\mathbf{x}]] \times (U\rho_{\kappa}\mathbf{v}^{\pm} + \mathbf{P}^{\pm}\mathbf{N}_s) = \mathbf{0}, \quad (2.156)$$

where the superscript  $\pm$  indicates that either of the limits can be used. For a motion which is continuous across the singular surface, i.e.  $[[\mathbf{x}]] = \mathbf{0}$ , this results into a trivial relation, and therefore is of no consequence. But for  $[[\mathbf{x}]] \neq \mathbf{0}$ , (2.156) provides us with an additional jump condition to be satisfied across the singular surface.

The corresponding spatial form of the equation (2.153) is

$$\mathbf{T} = \mathbf{T}^T. \quad (2.157)$$

*Remark 2.2.3.* The balance of angular momentum implies the balance of linear momentum.

Let  $\mathbf{c}$  be an arbitrary vector. Rewrite equation (2.151) after replacing  $\mathbf{x}_0$  by  $(\mathbf{x}_0 + \mathbf{c})$ .

Subtract (2.151) from this equation to get

$$\frac{d}{dt} \int_{\Omega} \rho_{\kappa} \mathbf{c} \times \mathbf{v} dV = \int_{\partial\Omega} \mathbf{c} \times \mathbf{p} dA + \int_{\Omega} \rho_{\kappa} \mathbf{c} \times \mathbf{b} dV. \quad (2.158)$$

Since  $\mathbf{c}$  is arbitrary, we get the desired result.

**Balance of energy** We restrict our attention to systems where the energy is supplied to the body either through mechanical work (done by contact and body forces) or via a supply of heat. We assume that the supply of heat to  $\mathfrak{S}$  has two sources. The *contact heating* supplied to  $\mathfrak{S}_1$  by  $\mathfrak{S}_2$  through their surface of contact is

$$H_c(\mathfrak{S}_1, \mathfrak{S}_2, t) = \int_I q dA = \int_i h da, \quad (2.159)$$

where  $q \in \mathbb{R}$  and  $h \in \mathbb{R}$  are heat flux per unit area of  $I = \kappa(\mathfrak{S}_1) \cap \kappa(\mathfrak{S}_2)$  and  $i = \chi(\mathfrak{S}_1) \cap \chi(\mathfrak{S}_2)$ , respectively. The *external supply of heat* to  $\mathfrak{S}$  is received from sources external to the body and is given by

$$H_e(\mathfrak{S}, t) = \int_{\Omega} \rho_{\kappa} r dV = \int_{\omega} \rho r dv, \quad (2.160)$$

where  $r = \hat{r}(\mathbf{X}, t) = \tilde{r}(\mathbf{x}, t)$  is the rate of heat supply to  $\mathfrak{S}$  per unit mass of  $\mathfrak{S}$ . Therefore, the total heat supply to  $\mathfrak{S}$  is

$$H(\mathfrak{S}, t) = H_c(\mathfrak{S}, \mathfrak{B} \setminus \mathfrak{S}, t) + H_e(\mathfrak{S}, t). \quad (2.161)$$

The total energy  $U$  of the part  $\mathfrak{S}$  of the body at any time consists of the kinetic energy and the internal energy of  $\mathfrak{S}$

$$U(\mathfrak{S}, t) = \int_{\Omega} \frac{1}{2} \rho_{\kappa} \mathbf{v} \cdot \mathbf{v} dV + \int_{\Omega} \rho_{\kappa} e dV, \quad (2.162)$$

where  $e$  is the internal energy per unit mass of  $\mathfrak{S}$ . The balance of total energy is the *first law of thermodynamics* which postulates that a time-change in total energy of  $\mathfrak{S}$  is balanced by the supply of the mechanical power and the heat to (or from)  $\mathfrak{S}$ :

$$\dot{U}(\mathfrak{S}, t) = P(\mathfrak{S}, t) + H(\mathfrak{S}, t), \quad (2.163)$$

where the mechanical power  $P$  is of the form

$$P(\mathfrak{S}, t) = \int_{\partial\Omega} \mathbf{p} \cdot \mathbf{v} dA + \int_{\Omega} \rho_{\kappa} \mathbf{b} \cdot \mathbf{v} dV. \quad (2.164)$$

Upon substituting definitions (2.162), (2.164), and (2.161) into (2.163) we obtain the referential form of the balance of energy

$$\frac{d}{dt} \int_{\Omega} \rho_{\kappa} \left( e + \frac{1}{2} |\mathbf{v}|^2 \right) dV = \int_{\partial\Omega} (\mathbf{v} \cdot \mathbf{P}\mathbf{N} + q) dA + \int_{\Omega} \rho_{\kappa} (\mathbf{v} \cdot \mathbf{b} + r) dV. \quad (2.165)$$

By Noll's and Cauchy's theorems, the balance law (2.165) implies the existence of a vector  $\mathbf{q}$  such that  $q = -\mathbf{q} \cdot \mathbf{N}$  (the  $-$  sign is conventional). The vector  $\mathbf{q}$  is the referential heat flux vector (we can similarly argue for the existence of a vector  $\mathbf{h}$ , the spatial heat flux vector, such that  $h = -\mathbf{h} \cdot \mathbf{n}$ ). The local form of the balance of energy can be obtained upon using the transport theorem (2.113), the divergence theorem (2.97), and the localization theorem.

We get

$$\rho_{\kappa} \left( e + \frac{1}{2} |\mathbf{v}|^2 \right) \dot{\phantom{x}} = \text{Div}(\mathbf{P}^T \mathbf{v} - \mathbf{q}) + \rho_{\kappa} (\mathbf{v} \cdot \mathbf{b} + r) \quad (2.166)$$

outside the singular surface and

$$-U\rho_\kappa\left[e + \frac{1}{2}|\mathbf{v}|^2\right] = \llbracket \mathbf{P}^T \mathbf{v} - \mathbf{q} \rrbracket \cdot \mathbf{N}_s \quad (2.167)$$

on the singular surface  $S_t$  (the conditions for mass balance, (2.129) and (2.130), have also been used). These two equations, on using the local forms of the balance of linear momentum, reduce to

$$\rho_\kappa \dot{e} = \mathbf{P} \cdot \dot{\mathbf{F}} - \text{Div } \mathbf{q} + \rho_\kappa r \quad (2.168)$$

and

$$U\rho_\kappa\llbracket e \rrbracket = -\llbracket \mathbf{v} \rrbracket \cdot \langle \mathbf{P} \rangle \mathbf{N}_s + \llbracket \mathbf{q} \rrbracket \cdot \mathbf{N}_s, \quad (2.169)$$

respectively. For a coherent interface, use (2.74) to rewrite (2.169) as

$$U\rho_\kappa\llbracket e \rrbracket = U\langle \mathbf{P} \rangle \cdot \llbracket \mathbf{F} \rrbracket + \llbracket \mathbf{q} \rrbracket \cdot \mathbf{N}_s. \quad (2.170)$$

The spatial form of these balance equations can be derived in a similar manner.

We obtain

$$\rho \dot{e} = \mathbf{T} \cdot \dot{\mathbf{L}} - \text{div } \mathbf{h} + \rho r \quad (2.171)$$

outside the singular surface  $s_t$  in  $\chi(\mathfrak{B})$  and

$$-j_s\llbracket e \rrbracket = \langle \mathbf{T} \rangle \llbracket \mathbf{v} \rrbracket \cdot \mathbf{n}_s - \llbracket \mathbf{h} \rrbracket \cdot \mathbf{n}_s \quad (2.172)$$

on the singular surface  $s_t$ .

*Remark 2.2.4.* The balance of mass and momentum follows from the balance of energy.<sup>3</sup>

To obtain the balance of mass, recall Galileo's *law of inertia* (also called Newton's first

---

<sup>3</sup>This assertion was first made by Green and Rivlin [62] using invariance under superimposed rigid body motions. Another argument based on material frame indifference was later provided by Šilhavý ([156], Ch. 6). Our discussion is motivated from the symmetries of classical physics and does not (explicitly) require principles of rigid body invariance and material frame indifference.

law of motion): the body in the state of uniform motion (i.e.  $\mathbf{v} = \mathbf{c}$ , a constant) remains so, unless an external force is applied to it. It is also assumed that no heat is exchanged with the body (which otherwise might bring a change in the state even during a uniform motion). We apply this law to  $\Omega$  with zero applied force ( $\mathbf{p} = \mathbf{0} = \mathbf{b}$ ), no heat supply and constant velocity  $\mathbf{c}$ . Since the internal energy is a function of the state of the body, it remains unchanged during the uniform motion. The global balance of energy (2.165) then implies

$$\frac{1}{2}|\mathbf{c}|^2 \frac{d}{dt} \int_{\Omega} \rho_{\kappa} dV = 0, \quad (2.173)$$

which reduces to the global form of the balance of mass (2.127), since  $\mathbf{c}$  is an arbitrary constant.

The balance of linear momentum is recovered if we assume that for all inertial frames of reference (velocity under such frames are related by  $\mathbf{v}' = \mathbf{v} + \mathbf{c}$ , with constant  $\mathbf{c}$ ), quantities  $\rho_{\kappa}e$ ,  $\mathbf{p}$ ,  $\mathbf{b}$ ,  $q$  and  $r$  remain invariant. Assume that the balance of energy (2.165) is written for an inertial frame. For another inertial frame, where the velocity field is  $\mathbf{v}' = \mathbf{v} + \mathbf{c}$ , the balance law takes the following form

$$\frac{d}{dt} \int_{\Omega} \rho_{\kappa} \left( e + \frac{1}{2} |\mathbf{v} + \mathbf{c}|^2 \right) dV = \int_{\partial\Omega} ((\mathbf{v} + \mathbf{c}) \cdot \mathbf{PN} + q) dA + \int_{\Omega} \rho_{\kappa} ((\mathbf{v} + \mathbf{c}) \cdot \mathbf{b} + r) dV. \quad (2.174)$$

Subtracting relation (2.165) from (2.174), and using (2.173), we get

$$\frac{d}{dt} \int_{\Omega} \rho_{\kappa} \mathbf{c} \cdot \mathbf{v} dV = \int_{\partial\Omega} \mathbf{c} \cdot \mathbf{PN} dA + \int_{\Omega} \rho_{\kappa} \mathbf{c} \cdot \mathbf{b} dV. \quad (2.175)$$

As  $\mathbf{c}$  is an arbitrary constant, this relation reduces to the balance of linear momentum (2.141).

We can recover the balance of angular momentum if we assume  $\rho_{\kappa}e$ ,  $\mathbf{p}$ ,  $\mathbf{b}$ ,  $q$  and  $r$  to be invariant for any frame of reference (infinitesimally) rotating with respect to an inertial

frame such that  $\mathbf{v}' = \mathbf{v} + \boldsymbol{\omega} \times (\mathbf{x} - \mathbf{x}_0)$ , where  $\mathbf{v}$  is the velocity field in an inertial frame of reference. The vector  $\boldsymbol{\omega} \in \mathcal{V}_\chi$  is an arbitrary (constant) angular velocity and  $\mathbf{x}_0 \in \mathcal{E}_\chi$  is any fixed point. Writing the balance of energy for a reference frame which is rotating with respect to the inertial frame, for which the balance law (2.165) holds, we obtain

$$\begin{aligned} \frac{d}{dt} \int_{\Omega} \rho_\kappa \left( e + \frac{1}{2} |\mathbf{v} + \boldsymbol{\omega} \times (\mathbf{x} - \mathbf{x}_0)|^2 \right) dV &= \int_{\partial\Omega} ((\mathbf{v} + \boldsymbol{\omega} \times (\mathbf{x} - \mathbf{x}_0)) \cdot \mathbf{PN} + q) dA \\ &+ \int_{\Omega} \rho_\kappa ((\mathbf{v} + \boldsymbol{\omega} \times (\mathbf{x} - \mathbf{x}_0)) \cdot \mathbf{b} + r) dV. \end{aligned} \quad (2.176)$$

After subtracting (2.165) from (2.176) and rearranging the integrands we obtain

$$\begin{aligned} \frac{d}{dt} \int_{\Omega} \rho_\kappa (\boldsymbol{\omega} \cdot (\mathbf{x} - \mathbf{x}_0) \times \mathbf{v} + \frac{1}{2} |\boldsymbol{\omega} \times (\mathbf{x} - \mathbf{x}_0)|^2) dV &= \int_{\partial\Omega} \boldsymbol{\omega} \cdot (\mathbf{x} - \mathbf{x}_0) \times \mathbf{PN} dA \\ &+ \int_{\Omega} \rho_\kappa \boldsymbol{\omega} \cdot (\mathbf{x} - \mathbf{x}_0) \times \mathbf{b} dV. \end{aligned} \quad (2.177)$$

Let  $\boldsymbol{\omega} = \epsilon \boldsymbol{\omega}_1$ , where  $\epsilon \in \mathbb{R}$  and  $\boldsymbol{\omega}_1 \in \mathcal{V}_\chi$  are constant. Substitute this in (2.177), divide the whole equation by  $\epsilon$  and let  $\epsilon \rightarrow 0$ . Obtain

$$\boldsymbol{\omega}_1 \cdot \frac{d}{dt} \int_{\Omega} \rho_\kappa (\mathbf{x} - \mathbf{x}_0) \times \mathbf{v} dV = \boldsymbol{\omega}_1 \cdot \int_{\partial\Omega} (\mathbf{x} - \mathbf{x}_0) \times \mathbf{PN} dA + \boldsymbol{\omega}_1 \cdot \int_{\Omega} \rho_\kappa (\mathbf{x} - \mathbf{x}_0) \times \mathbf{b} dV. \quad (2.178)$$

The balance of angular momentum (2.151) is then recovered from (2.178) on using the arbitrariness of  $\boldsymbol{\omega}_1$ . Substitute the result into (2.177) to get

$$\frac{d}{dt} \int_{\Omega} \rho_\kappa |\boldsymbol{\omega} \times (\mathbf{x} - \mathbf{x}_0)|^2 dV = 0, \quad (2.179)$$

which can be rewritten as (since  $\boldsymbol{\omega}$  is constant)

$$\boldsymbol{\omega} \cdot \frac{d\mathbf{I}_{x_0}}{dt} \boldsymbol{\omega} = 0, \quad (2.180)$$



where

$$\mathbf{I}_{x_0} = \int_{\Omega} \rho_{\kappa} (|\mathbf{x} - \mathbf{x}_0|^2 \mathbf{1} - (\mathbf{x} - \mathbf{x}_0) \otimes (\mathbf{x} - \mathbf{x}_0)) dV \quad (2.181)$$

is the inertia tensor ([81], page 496), a quantity in rotational dynamics analogous to mass in translational dynamics. Note that  $\mathbf{I}_{x_0}$  is symmetric and thus can be diagonalized. Using the arbitrariness of the constant  $\boldsymbol{\omega}$ , it then follows from (2.180) that

$$\frac{d\mathbf{I}_{x_0}}{dt} = 0, \quad (2.182)$$

i.e. the inertia tensor (with respect to the rotating frame) is time independent.

### 2.2.3 Clausius-Duhem inequality

The *state* of a material point is a set of variables, assumed to characterize it uniquely. The set of variables can be divided into two groups: one which define the state of motion (velocities) and the other, which define the thermodynamic state of the material point (stress, strain, temperature, specific energy, etc.). In this thesis, however, a state would, in general, refer to the thermodynamic state (cf. [18], page 126). The state of body  $\mathfrak{B}$  is the collection of states of the constituting material points. A material point is in the *equilibrium state* if it remains in the same state under vanishing external influence.

During an irreversible process, the body evolves asymmetrically in time. In other words, a process which takes the body (or a part of it) from state  $A$  to state  $B$ , is *irreversible*, if on reversing the direction of time (i.e. reversing the sign of the time variable in the equations which describe the process), it fails to take the body from state  $B$  to state  $A$ . Therefore, irreversible processes can be characterized with a preferred direction in time. The purpose of the second law of thermodynamics is to prescribe this preferred direction.

Classically, the second law has been formulated in terms of equilibrium states and reversible processes [142]. Its extension to non-equilibrium states and irreversible processes has been a subject of much debate for more than a century now.<sup>4</sup> Central to the discussion is the question of the existence of quantities like absolute temperature, energy, and entropy outside equilibrium. This problem was initially addressed by the Brussels school of thermodynamics (De Donder, Prigogine, etc.) using the concept of *local equilibrium* [146, 87], under which the notions of temperature, energy, and entropy, are assumed to make sense, if only locally.<sup>5</sup> In the past fifty years many more attempts have been made to provide a *rational* theory of irreversible thermodynamics. In particular, we note the work done by Truesdell, Coleman, Serrin, Owen, and Šilhavý.<sup>6</sup> Our assumption, therefore, of existence of a temperature field, specific energy density, and specific entropy density, rests on rigorous grounds, valid for a sufficiently wide class of irreversible processes. We will take up this discussion again, in the context of plasticity, in Chapter 3.

To this end, we consider the statement of the second law of thermodynamics as: the evolution proceeds so as to always bring a non-decreasing change in the internal entropy of the body [146]. We assume the existence of specific entropy  $\eta \in \mathbb{R}$  such that the total entropy  $s$  (in the reference configuration) is given by

$$s = \int_{\Omega} \rho_{\kappa} \eta dV. \quad (2.183)$$

---

<sup>4</sup>The situation is aptly described by Bridgman [18] in the opening sentence of his discussion on the second law of thermodynamics: “There has been nearly as many formulations of the second law as there have been discussions of it”.

<sup>5</sup>By a *local* region, Prigogine [146] meant a macroscopic region containing enough molecules for microscopic fluctuations to be negligible. In our context, such local regions are represented by material points.

<sup>6</sup>Two excellent collection of articles outlining their (and related) ideas are [169] and [154].

A change in the total entropy is due to the change in the external entropy ( $s_e$ ) and the change in the internal entropy ( $s_i$ ). We write

$$\dot{s} = \dot{s}_e + \dot{s}_i. \quad (2.184)$$

The change in the external entropy represents the change in entropy of the sub-body  $\Omega$  as a result of its interaction with the surroundings. For a diffusion-less process it is given by [146, 154]

$$\dot{s}_e = \int_{\partial\Omega} \frac{q}{\theta} dA + \int_{\Omega} \rho_{\kappa} \frac{r}{\theta} dV, \quad (2.185)$$

where  $\theta > 0$  is the absolute temperature. According to the second law

$$\dot{s}_i \geq 0, \quad (2.186)$$

with equality holding for a reversible process. This can be rewritten in the form of the Clausius-Duhem inequality, using equations (2.183)-(2.185) as [156]

$$\frac{d}{dt} \int_{\Omega} \rho_{\kappa} \eta dV \geq \int_{\partial\Omega} \frac{q}{\theta} dA + \int_{\Omega} \rho_{\kappa} \frac{r}{\theta} dV. \quad (2.187)$$

Use the transport theorem (2.113) and the divergence theorem (2.97) to obtain the local forms

$$\rho_{\kappa} \dot{\eta} \geq -\text{Div} \frac{\mathbf{q}}{\theta} + \rho_{\kappa} \frac{r}{\theta} \quad (2.188)$$

outside the singular surface and

$$-U \rho_{\kappa} \llbracket \eta \rrbracket \geq - \left[ \left[ \frac{\mathbf{q}}{\theta} \right] \right] \cdot \mathbf{N}_s \quad (2.189)$$

on the singular surface. The balance of mass and the relation  $q = -\mathbf{q} \cdot \mathbf{N}$  have also been used in obtaining these local inequalities. Use the balance of energy (2.168) to eliminate  $r$

from (2.188). Obtain

$$\rho_\kappa \theta \dot{\eta} \geq \rho_\kappa \dot{e} - \mathbf{P} \cdot \dot{\mathbf{F}} - \theta \operatorname{Div} \frac{\mathbf{q}}{\theta} + \operatorname{Div} \mathbf{q}. \quad (2.190)$$

By the chain rule of differentiation

$$\operatorname{Div} \frac{\mathbf{q}}{\theta} = \frac{\operatorname{Div} \mathbf{q}}{\theta} - \frac{\mathbf{q} \cdot \mathbf{g}}{\theta^2}, \quad (2.191)$$

with  $\mathbf{g} = \nabla \theta$ . Inequality (2.190) can then be rewritten as

$$\rho_\kappa \theta \dot{\eta} \geq \rho_\kappa \dot{e} - \mathbf{P} \cdot \dot{\mathbf{F}} + \frac{\mathbf{q} \cdot \mathbf{g}}{\theta}. \quad (2.192)$$

Similarly, we can eliminate  $[[\mathbf{q}/\theta]] \cdot \mathbf{N}_s$  between (2.170) and (2.189). Use (2.46) to write

$$[[\mathbf{q}]] = \langle \theta \rangle \left[ \left[ \frac{\mathbf{q}}{\theta} \right] \right] + [[\theta]] \left\langle \frac{\mathbf{q}}{\theta} \right\rangle. \quad (2.193)$$

Substituting this in (2.189) and eliminating  $[[\mathbf{q}]] \cdot \mathbf{N}_s$  from (2.170) yields

$$-U \rho_\kappa \langle \theta \rangle [[\eta]] \geq -U(\rho_\kappa [[e]] - \langle \mathbf{P} \rangle \cdot [[\mathbf{F}]]) + [[\theta]] \left\langle \frac{\mathbf{q}}{\theta} \right\rangle \cdot \mathbf{N}_s. \quad (2.194)$$

Define specific free energy density as

$$f = e - \theta \eta. \quad (2.195)$$

Therefore

$$\dot{f} = \dot{e} - \dot{\theta} \eta - \theta \dot{\eta} \quad (2.196)$$

and

$$[[f]] = [[e]] - \langle \theta \rangle [[\eta]] - [[\theta]] \langle \eta \rangle. \quad (2.197)$$

It is then straightforward to rewrite equations (2.192) and (2.194) in terms of the free energy density. Substitute  $\dot{e}$  and  $[[e]]$  from (2.196) and (2.197), respectively, into equations (2.192) and (2.194) to obtain

$$\rho_\kappa \dot{f} - \mathbf{P} \cdot \dot{\mathbf{F}} + \rho_\kappa \eta \dot{\theta} + \frac{\mathbf{q} \cdot \mathbf{g}}{\theta} \leq 0 \quad (2.198)$$

and

$$U(\rho_\kappa \llbracket f \rrbracket - \langle \mathbf{P} \rangle \cdot \llbracket \mathbf{F} \rrbracket) + (U\rho_\kappa \langle \eta \rangle - \left\langle \frac{\mathbf{q}}{\theta} \right\rangle \cdot \mathbf{N}_s) \llbracket \theta \rrbracket \geq 0. \quad (2.199)$$

Use (2.46) to write

$$\mathbf{N}_s \cdot \llbracket \mathbf{F}^T \mathbf{P} \rrbracket \mathbf{N}_s = \llbracket \mathbf{F} \rrbracket \mathbf{N}_s \cdot \langle \mathbf{P} \rangle \mathbf{N}_s + \langle \mathbf{F} \rangle \mathbf{N}_s \cdot \llbracket \mathbf{P} \rrbracket \mathbf{N}_s. \quad (2.200)$$

Furthermore, compatibility (2.65) implies that  $\mathbf{N}_s \otimes \llbracket \mathbf{F} \rrbracket \mathbf{N}_s = \llbracket \mathbf{F}^T \rrbracket$  and therefore

$$\llbracket \mathbf{F} \rrbracket \mathbf{N}_s \cdot \langle \mathbf{P} \rangle \mathbf{N}_s = \text{tr}\{\langle \mathbf{P} \rangle (\mathbf{N}_s \otimes \llbracket \mathbf{F} \rrbracket \mathbf{N}_s)\} = \text{tr}(\langle \mathbf{P} \rangle \llbracket \mathbf{F}^T \rrbracket) = \langle \mathbf{P} \rangle \cdot \llbracket \mathbf{F} \rrbracket. \quad (2.201)$$

Also, using the balance of linear momentum at the surface (2.144), the compatibility condition (2.74), and the identity (2.46), we get

$$\langle \mathbf{F} \rangle \mathbf{N}_s \cdot \llbracket \mathbf{P} \rrbracket \mathbf{N}_s = -U\rho_\kappa \langle \mathbf{F} \rangle \mathbf{N}_s \cdot \llbracket \mathbf{v} \rrbracket = U^2 \rho_\kappa \langle \mathbf{F} \rangle \mathbf{N}_s \cdot \llbracket \mathbf{F} \rrbracket \mathbf{N}_s = \frac{1}{2} U^2 \rho_\kappa \llbracket |\mathbf{F} \mathbf{N}_s|^2 \rrbracket. \quad (2.202)$$

Substituting (2.202) and (2.201) into (2.200) we obtain

$$\mathbf{N}_s \cdot \llbracket \mathbf{F}^T \mathbf{P} \rrbracket \mathbf{N}_s = \langle \mathbf{P} \rangle \cdot \llbracket \mathbf{F} \rrbracket + \frac{1}{2} U^2 \rho_\kappa \llbracket |\mathbf{F} \mathbf{N}_s|^2 \rrbracket. \quad (2.203)$$

Thus (2.199) can be rewritten as

$$U \left( \mathbf{N}_s \cdot \llbracket \mathbf{E} \rrbracket \mathbf{N}_s + \frac{1}{2} U^2 \rho_\kappa \llbracket |\mathbf{F} \mathbf{N}_s|^2 \rrbracket \right) + \left( U\rho_\kappa \langle \eta \rangle - \left\langle \frac{\mathbf{q}}{\theta} \right\rangle \cdot \mathbf{N}_s \right) \llbracket \theta \rrbracket \geq 0, \quad (2.204)$$

where

$$\mathbf{E} = \rho_\kappa f \mathbf{1} - \mathbf{F}^T \mathbf{P} \quad (2.205)$$

is the Eshelby tensor.<sup>7</sup>

---

<sup>7</sup>Named after J. D. Eshelby, whose work has had great impact in many areas of defect mechanics. A collection of all his published work is now available [116].

## Chapter 3

# A Continuum Theory of Plastic

# Deformation<sup>1</sup>

In this chapter we lay down a thermodynamically consistent theory of plastic evolution in solids. By *plastic evolution* (or plastic flow) we understand an irreversible deformation process, which brings permanent structural changes in a solid. In our treatment we assume such permanent changes to be brought either via motion of dislocations [38] (e.g. slip) or as a result of a moving interface (e.g. twin boundaries [36], surface dislocations [13]). In the present (and the following) chapter, we will mainly concentrate on plastic deformation in the bulk, away from the interface. Our discussion on the thermodynamics of plastic flow, will however be general, except that we include an interface energy term only in Chapter 6.

That dislocations are carriers of plasticity, at least in crystals, was reported in 1934 in the independent works of Orowan [136], Polanyi [144], and Taylor [162]. The paper by

---

<sup>1</sup>A few sections of this chapter have appeared in a recent research article [66].

Taylor, in addition, pioneered the study of work hardening in crystals (see the first remark in Section 3.8). These works emphasized the microscopic nature of plastic flow, which unlike (conventional) elasticity is a consequence of microstructural rearrangements and therefore always inhomogeneous, at least locally. A homogeneous plastic flow can be understood only as an average over a macroscopic region. The phenomenological theory of plasticity, on the other hand, developed independently as a subject of macroscopic observations (and predictions) of plastic flow. Such a theory has of course been motivated by imminent engineering challenges and experimental limitations. Its development in metals can be traced back to as far as 1864, when Tresca published his studies of a yield criteria for initiating plastic flow. Significant progress in the subject was subsequently made by Saint-Venant, Lévy, von Mises, Hencky, Prandtl, Reuss, Nadai, Schmidt and Hill (for a detailed historical outline, see [75]). The study of plastic flow as a thermodynamically irreversible process appears to have begun in the works of Eckart [44] and Bridgman [20]. This resulted in an attempt to precisely understand the evolution of plastic flow in a sufficiently general thermodynamic environment. As we shall see below, thermodynamics provides us with a natural starting point for the development of the theory. By 1950, plasticity had achieved a status of one of the most challenging problems in condensed matter physics, continuum mechanics and thermodynamics. The theory, as developed in the next two chapters, combines various ideas from microscopic, macroscopic and as well as thermodynamic viewpoints to present a coherent picture of plastic flow.

The modern literature on metal plasticity emphasizes a multiplicative decomposition of the deformation gradient into elastic and plastic factors in which the former measures

distortion relative to some unstressed or *relaxed* configuration of a local neighborhood of a material point. The definition of the elastic deformation in terms of information about the stress immediately implies that the former is inherently both constitutive and kinematic in nature. This contrasts with conventional ideas in continuum theory according to which kinematical and dynamical variables are viewed as being conceptually independent of a constitutive framework. The constitutive/geometric nature of the constituent elastic and plastic deformations affords considerable latitude in resolving ambiguities about their properties that are unavoidable in a purely geometric interpretation. We will extract definitive statements about these variables from specific constitutive hypotheses and thus clarify the structure of initial-boundary-value problems for the motion of a continuum in the presence of plasticity.

The basis of the idea of a local stress-free state, and an associated manifold of intermediate configurations, is examined in Section 3.1. This is grounded in the notion of an equilibrium unloading process together with appropriate constitutive hypotheses on the elastic response. In Section 3.2 the constituent elastic and plastic deformations are discussed. Stokes' theorem is used to describe the concepts of incompatibility and the associated dislocation density. The notion of geometrically necessary and statistically stored dislocation densities is also clarified. In Section 3.3, restrictions are obtained for a constitutive function to be independent of compatible changes in the reference configuration. The basis for such an invariance is the fact that our choice of a reference configuration is arbitrary and therefore should not have any influence on the material response. The basic thermodynamic framework is discussed in Section 3.4, where the elasticity of the body is



described and the dissipation associated with the plastic evolution is expressed in terms of Eshelby's tensor. Of central importance is the assumption introduced there of strong dissipation, according to which plastic evolution is inherently dissipative. This imposes a constraint on the kinds of evolution that qualify as plasticity, constituting, in effect, part of the definition of plastic flow. It is used, in Section 3.5, to derive unambiguous transformation rules for the elastic and plastic deformations under superposed rigid-body motions. Material symmetry restrictions on the elastic response and on constitutive equations for yield and plastic flow are discussed in Sections 3.6 and 3.7, following ideas put forth in [168] and [45]. In Section 3.7, the latitude afforded by the constitutive character of the plastic deformation is used to dispose of a long-standing controversy surrounding plastic spin. Finally, in section 3.8, we provide some remarks on work hardening, size effects, symmetry groups and Bauschinger effect.

We use the notation from Chapter 2 and denote  $\kappa_r \equiv \boldsymbol{\kappa}(\mathfrak{B})$  and  $\kappa_t \equiv \boldsymbol{\chi}(\mathfrak{B})$  as the placements of the body  $\mathfrak{B}$  in a (global) fixed reference configuration and a (global) spatial configuration, respectively. As in Chapter 2, a piecewise continuously differentiable map is assumed to relate these two global configurations.

### 3.1 Unloading elastic bodies to zero stress

A central tenet of the considered model is the idea that stress is purely elastic in origin, the associated deformation being measured from a stress-free local configuration. It

is therefore of no small importance to justify this assumption.<sup>2</sup> To explore this issue we appeal to the mean-stress theorem, according to which the mean Cauchy stress in a body is zero if it is in equilibrium and subjected to vanishing surface tractions and body forces.<sup>3</sup> Thus, the mean stress for some  $\omega \subset \kappa_t$  (such that  $\omega \cap s_t = \emptyset$ )

$$\bar{\mathbf{T}}(t) = (\text{vol}(\omega))^{-1} \int_{\omega} \mathbf{T}(\mathbf{x}, t) dv \quad (3.1)$$

vanishes, where  $\mathbf{T}$  is the Cauchy stress,  $\text{vol}(\omega)$  is the volume of a part  $\omega$  of the configuration  $\kappa_t$ . This theorem is valid for stress fields that are differentiable and hence continuous in  $\omega$ . The mean-value theorem is then applicable and guarantees the existence of  $\bar{\mathbf{x}} \in \omega$  such that  $\mathbf{T}(\bar{\mathbf{x}}, t) = \bar{\mathbf{T}}$  ( $= \mathbf{0}$ ). Let

$$d(\kappa_t) = \sup_{\mathbf{x}, \mathbf{y} \in \omega} |\mathbf{x} - \mathbf{y}| \quad (3.2)$$

be the diameter of  $\omega$ . For  $d \rightarrow 0$  we have  $|\mathbf{x} - \bar{\mathbf{x}}| \rightarrow 0$  for all  $\mathbf{x}$  in  $\omega$  and the continuity of  $\mathbf{T}(\mathbf{x}, t)$  furnishes  $\mathbf{T}(\mathbf{x}, t) \rightarrow \mathbf{T}(\bar{\mathbf{x}}, t) = \mathbf{0}$ . Thus, if the hypotheses of the mean-stress theorem are satisfied, then the local stress can be brought arbitrarily close to zero by making the diameter of the body correspondingly small against any length scale at hand. This result is of course independent of material constitution and furnishes theoretical justification for the measurement of residual stress by cutting out a small part of a body and observing its change in shape. Of course, this argument is not valid at the surface of singularity  $s_t$ , where the

---

<sup>2</sup>The arguments in this section are purely mechanical in nature, and therefore, for convenience, we suppress the dependence of fields on temperature.

<sup>3</sup>The mean Cauchy stress of a body in equilibrium can be calculated as: ([32], pages 105-106)

$$\bar{\mathbf{T}}(t) = \frac{1}{2} (\text{vol}(\omega))^{-1} \left\{ \int_{\omega} \rho(\mathbf{x} \otimes \mathbf{b} + \mathbf{b} \otimes \mathbf{x}) dv + \int_{\partial\omega} \rho(\mathbf{x} \otimes \mathbf{t} + \mathbf{t} \otimes \mathbf{x}) da \right\}.$$

Cauchy stress might suffer a discontinuity. However, such singular surfaces constitute a set of measure zero and therefore our argument remains valid *almost* everywhere in  $\kappa_t$ . We can in addition have a surface stress arising, for example, from a surface energy (as considered in Chapter 6). In that case, an appropriate argument can be made, for neighborhoods in the immediate vicinity of  $s_t$ , to relax the surface stress in addition to the bulk Cauchy stress. In the present section, we restrict our attention to the case when  $s_t = \emptyset$ , and postpone the discussion related of the interface until Chapters 5 and 6.

For elastic bodies the Cauchy stress is given in terms of the deformation from a configuration  $\kappa_i$  of  $\mathfrak{B}$  by (see Section 3.4)

$$J_H \mathbf{T} = W_{\mathbf{H}} \mathbf{H}^T, \quad (3.3)$$

where  $\mathbf{H}$  is the local map from the tangent space of  $\kappa_i$  to the tangent space  $\mathcal{V}$  of  $\kappa_t$  (at a material point),  $J_H (> 0)$  is the local ratio of volume in  $\kappa_t$  to that in  $\kappa_i$ , and  $W(\mathbf{H})$  is the strain energy per unit volume of  $\kappa_i$ . Here and henceforth we use bold subscripts to denote gradients with respect to tensors.<sup>4</sup> The function  $W(\mathbf{H})$  satisfies the requirement of frame invariance, in the sense that  $W(\mathbf{H}) = W(\mathbf{QH})$  for any rotation  $\mathbf{Q}$  (see the discussion given in Section 3.5), if and only if it is determined by the right Cauchy-Green deformation tensor  $\mathbf{C}_H = \mathbf{H}^T \mathbf{H}$ ; thus,  $W(\mathbf{H}) = \hat{W}(\mathbf{C}_H)$  and the relation  $W_{\mathbf{H}} = 2\mathbf{H}(\text{Sym} \hat{W}_{\mathbf{C}_H})$  furnishes

$$J_H \mathbf{T} = 2\mathbf{F} \left( \text{Sym} \hat{W}_{\mathbf{C}_H} \right) \mathbf{H}^T. \quad (3.4)$$

---

<sup>4</sup>The gradient of a scalar differentiable function  $G : \text{Lin} \rightarrow \mathbb{R}$  is the tensor  $G_{\mathbf{A}}$  defined by  $G(\mathbf{A} + \mathbf{B}) = G(\mathbf{A}) + G_{\mathbf{A}} \cdot \mathbf{B} + o(|\mathbf{B}|)$ , where  $\{\mathbf{A}, \mathbf{B}\} \in \text{Lin}$ . Moreover, if  $H$  is a differentiable function  $H : \text{Sym} \rightarrow \mathbb{R}$ , then its gradient is defined as the symmetric tensor  $\text{Sym}(H_{\mathbf{C}})$ , where  $\mathbf{C} \in \text{Sym}$ . To evaluate  $\text{Sym}(H_{\mathbf{C}})$ , consider an extension of  $H(\mathbf{C})$  from  $\text{Sym}$  to  $\text{Lin}$ . That is, define  $\bar{H}(\mathbf{C})$  for  $\mathbf{C} \in \text{Lin}$  such that  $\bar{H}(\mathbf{C}) = H(\mathbf{C})$  when  $\mathbf{C} \in \text{Sym}$ . The tensor  $\text{Sym}(H_{\mathbf{C}})$  is then given by  $\frac{1}{2} ((\bar{H}_{\mathbf{C}}) + (\bar{H}_{\mathbf{C}})^T)$ .

The Cauchy stress vanishes if and only if  $\hat{W}$  is stationary. Since  $\kappa_i$  is stress free,  $\hat{W}$  is stationary at  $\mathbf{C}_H = \mathbf{1}$ . We assume that  $\mathbf{C}_H = \mathbf{1}$  is the unique stationary point. This is assured by adopting the constitutive assumption that the strain-energy function is a strictly convex function of  $\mathbf{C}_H$  with a minimum at  $\mathbf{C}_H = \mathbf{1}$ . Thus, we assume that

$$\begin{aligned} \hat{W}(\mathbf{C}_{H_2}) - \hat{W}(\mathbf{C}_{H_1}) &> \text{Sym} \hat{W}_{\mathbf{C}_H}(\mathbf{C}_{H_1}) \cdot (\mathbf{C}_{H_2} - \mathbf{C}_{H_1}); \quad \mathbf{C}_{H_2} \neq \mathbf{C}_{H_1}, \\ \text{with } \hat{W}(\mathbf{1}) &= 0 \quad \text{and} \quad \text{Sym} \hat{W}_{\mathbf{C}_H}(\mathbf{1}) = \mathbf{0}. \end{aligned} \quad (3.5)$$

This in turn guarantees that stress relaxation is energetically optimal and reflects the phenomenology typical of metals in the elastic range provided that

$$|\mathbf{C}_H - \mathbf{1}| < \epsilon, \quad (3.6)$$

where  $\epsilon$  depends on the material at hand.

To elaborate, imagine cutting  $\kappa_t$  into an arbitrarily large number of sub-bodies of arbitrarily small diameter and relaxing the loads thereon. The mean-stress theorem together with our constitutive hypotheses imply that *equilibrium* states of these sub-bodies are stress-free, minimum-energy configurations in a Euclidean point space  $\mathcal{E}$  provided, as we assume here, that no energy is needed to generate the new surfaces created by this process. If these relaxed configurations cannot be made congruent in the absence of strain, then they do not fit together to form a connected whole in Euclidean space, and the material is then said to be *dislocated*. This then implies the non-existence of a global differentiable map from  $\kappa_t$  to the disjoint relaxed sub-bodies in  $\mathcal{E}$ . We thus relate the unstressed manifold to a smooth manifold  $\mathcal{M}$  which has a non-Euclidean structure (for more on smooth manifolds see [104]). The manifold  $\mathcal{M}$  is therefore the union of local configurations at each  $X \in \mathcal{B}$ . The local

configuration  $\kappa_i$  at  $X \in \mathfrak{B}$  can be identified with the tangent space  $T_{\mathcal{M}(p)}$  at  $p = \kappa_i(X)$ . Thus,  $\mathbf{H}$  locally maps  $\kappa_i$  at  $p = \kappa_i(X) \in \mathcal{M}$  to  $\mathcal{V}$  at  $\mathbf{x} = \boldsymbol{\chi}(X) \in \kappa_t$  and  $\mathbf{H}^T \mathbf{H}$  is the strain at  $p$  required to make the collection of stress-free sub-bodies in  $\mathcal{E}$  fit together in  $\kappa_t$ . The field  $\mathbf{H}$  does not then satisfy the usual compatibility condition which follows from the existence of a global differentiable map. The incompatibility is typically identified with a distribution of Burgers vectors via an analogy with the geometry of defective crystal lattices. This idea is the basis of the elegant differential-geometric theory of self-stressed bodies containing continuously distributed dislocations [44, 88, 14, 93, 129, 172, 99, 164, 90, 83]. Finally, note that both  $\mathcal{M}$  and  $\kappa_t$  might evolve with time, unlike  $\kappa_r$  which, by our choice, is fixed.

We now investigate a possible latitude offered by our constitutive assumptions on the nature of  $\kappa_i$ . Consider two relaxed configurations  $\kappa_{i_1}$  and  $\kappa_{i_2}$ . Let  $\mathbf{H}_1$  and  $\mathbf{H}_2$ , respectively, be the maps from the tangent space of these configurations to the translation space  $\mathcal{V}$  of  $\kappa_t$  at a spatial point  $\mathbf{x} \in \kappa_t$ . Thus

$$\mathbf{H}_1 = \mathbf{H}_2 \mathbf{A}, \quad (3.7)$$

where  $\mathbf{A}$ , with  $J_A > 0$ , is the map from the tangent space of  $\kappa_{i_1}$  to the tangent space of  $\kappa_{i_2}$  (or from  $\kappa_{i_1}$  to  $\kappa_{i_2}$ , since these local configurations are identified with their tangent spaces).

We wish to characterize any non-uniqueness in the local unloading process and so require that  $\mathbf{H}_1$  and  $\mathbf{H}_2$  generate the same Cauchy stress in  $\kappa_t$ :

$$(W_1)_{\mathbf{H}_1} (\mathbf{H}_1^*)^{-1} = \mathbf{T} = (W_2)_{\mathbf{H}_2} (\mathbf{H}_2^*)^{-1}, \quad (3.8)$$

where  $W_1(\mathbf{H}_1)$  and  $W_2(\mathbf{H}_2)$ , respectively, are the strain-energy functions based on  $\kappa_{i_1}$  and  $\kappa_{i_2}$ . These are related, modulo a constant, by

$$W_1(\mathbf{H}_1) = J_A W_2(\mathbf{H}_2). \quad (3.9)$$

To see this consider a parameterized path of deformations and let a superposed dot denote the derivative with respect to the parameter. Using  $\dot{W} = W_{\mathbf{H}} \cdot \dot{\mathbf{H}} = \mathbf{T}\mathbf{H}^* \cdot \dot{\mathbf{H}}$  with  $\mathbf{A}$  fixed, we then obtain

$$\dot{W}_1(\mathbf{H}_1) = \mathbf{T}\mathbf{H}_1^* \cdot \dot{\mathbf{H}}_1 = \mathbf{T}\mathbf{H}_2^* \mathbf{A}^* \cdot \dot{\mathbf{H}}_2 \mathbf{A} = \mathbf{T}\mathbf{H}_2^* \mathbf{A}^* \mathbf{A}^T \cdot \dot{\mathbf{H}}_2 = J_A \dot{W}_2(\mathbf{H}_2). \quad (3.10)$$

Integrating this with respect to the parameter we recover (3.9), modulo a constant.

The Cauchy stress vanishes at  $\mathbf{x}$  if and only if

$$\text{Sym}\{(\hat{W}_1)_{\mathbf{C}_{H_1}}\} = \mathbf{0} \quad \text{and} \quad \text{Sym}\{(\hat{W}_2)_{\mathbf{C}_{H_2}}\} = \mathbf{0}, \quad (3.11)$$

where

$$\hat{W}_1(\mathbf{C}_{H_1}) = J_A \hat{W}_2(\mathbf{C}_{H_2}) \quad \text{and} \quad \mathbf{C}_{H_1} = \mathbf{A}^T \mathbf{C}_{H_2} \mathbf{A}. \quad (3.12)$$

Our constitutive hypotheses, applied to both strain-energy functions, then imply that  $\mathbf{C}_{H_1} = \mathbf{C}_{H_2} = \mathbf{1}$  and hence that  $\mathbf{A}^T \mathbf{A} = \mathbf{1}$ . Thus,

$$\mathbf{A} \in \text{Orth}^+. \quad (3.13)$$

Substitution of (3.7) and (3.13) in (3.9) then yields

$$W_1(\mathbf{H}_1) = W_2(\mathbf{H}_1 \mathbf{A}^T). \quad (3.14)$$

We will assume our body to be materially uniform, i.e. assume that material at any two points in the body is same (see Remark 3.8.3 at the end of this chapter for a precise definition of material uniformity). In particular, the assumption of material uniformity ensures that  $W_1$  is not dependent explicitly on  $\mathbf{X}$ . Therefore,  $\mathbf{A}$  has to be uniform, since otherwise  $W_1$  will have a non-uniform character by virtue of (3.14). The unloading process therefore determines a local relaxed configuration modulo orientation and translation.

This degree of freedom is seen to follow directly from our constitutive hypotheses and the consequent interplay between deformation and stress in the definition of unloading.

Our assumption of a unique energy well in the domain of  $\hat{W}$  excludes certain models of crystal elasticity proposed by Ericksen [49] and Hill [74]. These models are motivated by the observation that there exist unimodular non-orthogonal transformations of a regular cubic lattice, say, which generate lattices that are geometric copies of each other. If  $W_1(\mathbf{H})$  and  $W_2(\mathbf{H})$  are the strain-energy functions for two lattices related in this manner, then it is natural to assume that they respond identically to a given deformation and thus that they satisfy the symmetry condition

$$W_1(\mathbf{H}) = W_2(\mathbf{H}). \quad (3.15)$$

Our view (see also [143]) is that symmetries of this kind do not fit naturally in the framework of Noll's simple elastic solid [128]. For, if  $\mathbf{G}$  is an element of the symmetry set of the first lattice, then by Noll's Rule  $\mathbf{K}\mathbf{G}\mathbf{K}^{-1}$  belongs to the symmetry set of the second, where  $\mathbf{K}$  is the gradient of the deformation that carries the first lattice to the second. We then have

$$W_1(\mathbf{H}) = W_1(\mathbf{H}\mathbf{G}) \quad \text{and} \quad W_2(\mathbf{F}) = W_2(\mathbf{H}\mathbf{K}\mathbf{G}\mathbf{K}^{-1}), \quad (3.16)$$

which imply that  $\mathbf{G} = \mathbf{K}$  and  $\mathbf{G} = \mathbf{K}^{-1}$  are symmetry transformations for both (hence all) lattices so related. Thus,

$$W(\mathbf{H}) = W(\mathbf{H}\mathbf{K}) = W(\mathbf{H}\mathbf{K}^{-1}), \quad (3.17)$$

where  $W$  stands for  $W_1$  or  $W_2$ . Let  $\mathbf{e}_i$  ( $i \in \{1, 2, 3\}$ ) be the axes of the first cubic lattice, normalized by the (uniform) lattice spacing and aligned with the edges of a typical cube. Then a transformation of the required type is furnished by the simple shear  $\mathbf{K} = \mathbf{1} + \gamma\mathbf{e}_1 \otimes \mathbf{e}_2$ ,

where  $\gamma$  is an integral multiple (positive or negative) of the lattice spacing. The inverse of  $\mathbf{K}$  is a simple shear of amount  $-\gamma$  and also furnishes a map of the lattice to itself. The presence of such  $\mathbf{K}$  and its inverse in the symmetry set is thus to be expected on physical grounds. In turn, this implies that  $\mathbf{K}^T \mathbf{C}_H \mathbf{K}$  belongs to the domain of the strain-energy function  $\hat{W}$  whenever  $\mathbf{C}_H$  does, for any amount of shear equal to an integral multiple (positive or negative) of the lattice spacing. Elastic response of this kind may be understood by regarding the bonds between atoms at the corners of a lattice cell as nonlinear springs. This analogy suggests that Noll's simple elastic material does not furnish an acceptable model of the physics at hand as arbitrarily large spring extensions would have to be admitted, whereas interatomic bonds presumably fail to persist when extended beyond finite limits.

Here, we discard the elastic interpretation and instead adopt the mechanism of plasticity to account for the underlying phenomenon. Thus, we re-interpret (3.15) as a statement to the effect that the *elastic* response of the lattice to a deformation  $\mathbf{H}$  is unaffected by *plastic* slip  $\mathbf{K}$  (or  $\mathbf{K}^{-1}$ ). We retain Noll's view insofar as a superposed elastic distortion  $\mathbf{H}$  is concerned. Variations in  $\mathbf{H}$  at fixed  $\mathbf{K}$  generate variations in stress in accordance with the elastic properties of the crystal, provided that such variations engender non-zero strains belonging to the domain of the elastic constitutive function. Thus, we introduce an elastic energy and confine symmetry transformations to subgroups of the orthogonal group, in accordance with Noll's original distinction between simple solids and simple fluids [128]. Such transformations preserve inequality (3.6) and the energy-minimizing value,  $\mathbf{1}$ , of  $\mathbf{C}_H$ . To model the invariance embodied in (3.15), it is then necessary to extend the constitutive structure beyond Noll's simple elastic solid to encompass the evolution of  $\mathbf{K}$ . This of course



is precisely the aim of Plasticity Theory. The shortcomings of Noll's simple materials as models of plasticity are discussed further in [130] and [147].

The connection between (3.17) and plasticity seems to be what Ball and James [8] have in mind in their discussion of lattice symmetry. Specifically, their view is that the domain of the strain-energy function should be limited in accordance with a restriction like (3.6) above so as to exclude from the symmetry group of the elastic response function the possibly large lattice shears typically associated with plasticity. The adjustment means that if  $\mathbf{C}_H$  belongs to the domain of  $\hat{W}$  then  $\mathbf{K}^T \mathbf{C}_H \mathbf{K}$  does not, if the amount of shear is sufficiently large. Instead, the latter would necessarily be associated with inelastic behavior. The restriction advocated by Ball and James excludes such shears from the theory of the elastic response of crystals. To effect such exclusion it is sufficient to assume (3.6) and to restrict the symmetry set to a subset of the orthogonal group.

## 3.2 Deformation and incompatibility

Let  $\mathbf{F}$  be the gradient of the deformation from  $\kappa_r$  to  $\kappa_t$  (cf. (2.21)). Let  $\mathbf{K}$  be the local map from tangent space  $\kappa_i$  to  $\mathcal{V}$  at  $\mathbf{X} \in \kappa_r$ . We assume  $J_K$  to be positive. Thus,  $\mathbf{H}$  and  $\mathbf{K}^{-1}$  are the *elastic* and *plastic* deformations, respectively. Unlike  $\mathbf{F}$ , they are not, in general, gradients of position fields. This issue is associated with the fact that position fields do not exist in  $\mathcal{M}$  due to its non-Euclidean character. We have<sup>5</sup> [91, 129, 103, 47]

$$\mathbf{H} = \mathbf{F}\mathbf{K}. \tag{3.18}$$

---

<sup>5</sup>A different notation, with  $\mathbf{F}^e$  in place of  $\mathbf{H}$  and  $\mathbf{F}^p$  in place of  $\mathbf{K}^{-1}$ , is usually found in the literature. We follow the notations introduced by Noll [129] and Epstein [47].

### 3.2.1 Dislocation density

The properties of the manifold  $\mathcal{M}$  imply that  $\text{Curl} \mathbf{K}^{-1}$  need not vanish. Let  $C \subset \kappa_r$  be a closed material curve, which bounds a surface  $A_C \subset \kappa_r$  (for every  $C$  there are infinitely many  $A_C$ ), with an associated unit normal  $\mathbf{N}$ . Define a vector  $\mathbf{B} \in T_{\mathcal{M}(p)}$  by

$$\mathbf{B}(C, t) \doteq \oint_C \mathbf{K}^{-1} d\mathbf{X} = \int_{A_C} (\text{Curl} \mathbf{K}^{-1})^T \mathbf{N} dA, \quad (3.19)$$

where the right-most equality follows if the field  $\mathbf{K}^{-1}$  is smooth (cf. (2.100)). This is referred to as the Burgers vector associated with  $C$  in recognition of its interpretation in dislocation theory. Thus, the existence of a non-zero Burgers vector is due to the incompatibility of the plastic deformation or, equivalently, to the non-existence of a position field in  $\mathcal{M}$  with (referential) gradient  $\mathbf{K}^{-1}$ . Using the (smooth) elastic deformation instead, we define vector  $\mathbf{b} \in T_{\mathcal{M}(p)}$  by

$$\mathbf{b}(c, t) \doteq \oint_c \mathbf{H}^{-1} d\mathbf{x} = \int_{A_c} (\text{curl} \mathbf{H}^{-1})^T \mathbf{n} da, \quad (3.20)$$

where  $c$  is the image of  $C \subset \kappa_r$  in  $\kappa_t$ , and  $A_c \subset \kappa_t$  is any surface bounded by  $c$  with unit-normal field  $\mathbf{n}(\mathbf{x}, t)$ . Recall from the definition of  $\mathbf{F}$ , that  $d\mathbf{x} = \mathbf{F}d\mathbf{X}$ . Substitute this in (3.20)<sub>1</sub> and use (3.18) and (3.19)<sub>1</sub> to conclude

$$\mathbf{b}(c, t) = \mathbf{B}(C, t), \quad (3.21)$$

a result which is valid even for piecewise smooth fields (considered in Section 5.1). Then  $\mathbf{H}^{-1}(\mathbf{x}, t)$  is incompatible if and only if  $\mathbf{K}^{-1}(\mathbf{X}, t)$  is incompatible. The tensors

$$\boldsymbol{\alpha}_r = \text{Curl} \mathbf{K}^{-1} \quad \text{and} \quad \boldsymbol{\alpha}_t = \text{curl} \mathbf{H}^{-1} \quad (3.22)$$

thus provide measures of the incompatibility per unit area of a material surface in  $\kappa_r$  and  $\kappa_t$ , respectively. Accordingly, we refer to these as the referential and spatial dislocation

densities.

In [30] an associated tensor  $\boldsymbol{\alpha}$  called the *true dislocation density*<sup>6</sup> is introduced.

This satisfies

$$J_K \mathbf{K}^{-1} \text{Curl} \mathbf{K}^{-1} = \boldsymbol{\alpha} = J_H \mathbf{H}^{-1} \text{curl} \mathbf{H}^{-1}, \quad (3.23)$$

wherein the outer equality may be shown to hold by first using Nanson's formula  $\mathbf{n} da = \mathbf{F}^* \mathbf{N} dA$  in (3.20)<sub>2</sub> and then using equations (2.25), (3.18), (3.21) and (3.19)<sub>2</sub> with the localization theorem for surfaces. The name is justified by the remarkable fact that  $\boldsymbol{\alpha}$  is invariant under arbitrary differentiable (i.e. compatible) variations of the configurations  $\kappa_r$  and  $\kappa_t$ . To see this we consider a variation of  $\kappa_r$  from  $\kappa_{r_1}$  to  $\kappa_{r_2}$  defined by the one-to-one map  $\mathbf{X}_2 = \boldsymbol{\lambda}(\mathbf{X}_1)$ , with invertible gradient  $\mathbf{A} = \nabla_1 \boldsymbol{\lambda}$ , where  $\nabla_1$  is the gradient with respect to  $\mathbf{X}_1$ . Using obvious notation we have  $\mathbf{K}_1^{-1} d\mathbf{X}_1 = \mathbf{K}_2^{-1} d\mathbf{X}_2$  and therefore

$$\int_{A_{C_2}} (\text{Curl}_2 \mathbf{K}_2^{-1})^T \mathbf{N}_2 dA_2 = \oint_{C_2} \mathbf{K}_2^{-1} d\mathbf{X}_2 = \oint_{C_1} \mathbf{K}_1^{-1} d\mathbf{X}_1 = \int_{A_{C_1}} (\text{Curl}_1 \mathbf{K}_1^{-1})^T \mathbf{N}_1 dA_1, \quad (3.24)$$

where  $C_2 = \boldsymbol{\lambda}(C_1)$ , provided that

$$\mathbf{K}_2 = \mathbf{A} \mathbf{K}_1. \quad (3.25)$$

Nanson's formula in the form  $\mathbf{N}_2 dA_2 = \mathbf{A}^* \mathbf{N}_1 dA_1$  and the arbitrariness of  $A_{C_1}$  then combine to give [30]

$$J_A \text{Curl}_2 \mathbf{K}_2^{-1} = \mathbf{A} \text{Curl}_1 \mathbf{K}_1^{-1}, \quad (3.26)$$

which yields the invariance of  $\boldsymbol{\alpha}$  by virtue of (3.23)<sub>1</sub> and  $J_{K_1} J_A = J_{K_2}$ . Further, (3.25) and (3.26) may be used with an obvious adjustment in notation to establish the outer equation in (3.23) directly. The same reasoning based on the second equality of (3.23)

---

<sup>6</sup>Teodosiu [164], however, refers to  $\boldsymbol{\alpha}_t$  as the true dislocation density.

proves the invariance of  $\alpha$  under arbitrary one-to-one differentiable variations of  $\kappa_t$ . In effect  $\alpha$  furnishes a measure of dislocation in the body *per se* in the sense that it is insensitive to the placement of the body in any configuration in  $\mathcal{E}$ . It is thus no coincidence that  $\alpha$  is associated with an intrinsic property of the material manifold  $\mathcal{M}$ , namely the *torsion* of the affine connection introduced by  $\mathbf{K}^{-1}$  and  $\nabla\mathbf{K}^{-1}$  (or  $\mathbf{H}^{-1}$  and  $\text{grad}\mathbf{H}^{-1}$ ) [129, 172].

### 3.2.2 Single dislocations

To obtain the representation of dislocation density and plastic distortion for a single dislocation, we follow Kunin [94, 95], and start by introducing a few generalized functions. Let  $L \subset \kappa_r$  be a material curve and let  $\phi(\mathbf{X})$  be a smooth scalar, vector or tensor field with bounded support on  $\kappa_r$ . The generalized function  $\delta(L)$  is then defined by

$$\int_{\kappa_r} \delta(L)\phi(\mathbf{X})dV = \int_L \phi(\mathbf{X}_L)dL, \quad (3.27)$$

where  $\mathbf{X}_L \in L$ . It then follows that

$$\delta(L) = \int_L \delta(\mathbf{X} - \mathbf{X}_L)dL, \quad (3.28)$$

where  $\delta(\mathbf{X} - \mathbf{X}_L)$  is the usual Dirac delta distribution. Equation (3.28) can be verified by substituting it into (3.27). We also introduce a surface generalized function. Let  $S \subset \kappa_r$  be a material surface. Define

$$\delta(S) = \int_S \delta(\mathbf{X} - \mathbf{X}_S)dS, \quad (3.29)$$

with  $\mathbf{X}_S \in S$ . This satisfies

$$\int_{\kappa_r} \delta(S)\phi(\mathbf{X})dV = \int_S \phi(\mathbf{X}_S)dS. \quad (3.30)$$

We can similarly define two vector valued generalized functions by

$$\int_{\kappa_r} \boldsymbol{\delta}(L)\phi(\mathbf{X})dV = \int_L \phi(\mathbf{X}_L)d\mathbf{L} \quad (3.31)$$

and

$$\int_{\kappa_r} \boldsymbol{\delta}(S)\phi(\mathbf{X})dV = \int_S \phi(\mathbf{X}_S)d\mathbf{S}, \quad (3.32)$$

where  $d\mathbf{L} = \mathbf{t}dL$  and  $d\mathbf{S} = \mathbf{N}dS$ , with  $\mathbf{t}$  being the unit tangent vector to  $L$ , and  $\mathbf{N}$ , the unit normal field associated with  $S$ . Let  $S$  be a surface bounded with curve  $L$ . Then [95]

$$\text{Curl } \boldsymbol{\delta}(S) = \boldsymbol{\delta}(L) \quad (3.33)$$

and therefore for a closed  $L$

$$\text{Div } \boldsymbol{\delta}(L) = 0. \quad (3.34)$$

Furthermore, note that, if  $L$  intersects  $S$  orthogonally at one point, say  $\mathbf{X}_0 \in \kappa_r$ , then we have<sup>7</sup>

$$\boldsymbol{\delta}(L) \cdot \boldsymbol{\delta}(S) = \delta(\mathbf{X} - \mathbf{X}_0). \quad (3.35)$$

Corresponding to a dislocation line (denoted by material curve  $L$ ) with unit tangent vector  $\mathbf{t} \in \mathcal{V}$  and Burgers vector  $\mathbf{b}$ , the dislocation density field  $\boldsymbol{\alpha}_r$  should then be such that for *any* closed curve  $C$  around  $L$ , the resulting Burgers vector (from equation (3.19)) should be a constant, i.e.  $\mathbf{b}$ . The following dislocation density distribution satisfies this requirement [89, 94, 95, 96]

$$\boldsymbol{\alpha}_r = \boldsymbol{\delta}(L) \otimes \mathbf{b}. \quad (3.36)$$

---

<sup>7</sup>Orthogonality requires that the tangent vector to the line  $L$  is parallel to the normal to the surface  $S$  at point  $\mathbf{X}_0 = L \cap S$ . The dot product of two generalized functions in (3.35) is well defined only if orthogonality holds at  $\mathbf{X}_0$ .

Indeed, on substituting (3.36) into the surface integral in (3.19), we obtain

$$\int_{A_C} \boldsymbol{\alpha}_r^T \mathbf{N} dA = \int_{\kappa_r} \boldsymbol{\alpha}_r^T \boldsymbol{\delta}(A_C) dV = \int_{\kappa_r} (\mathbf{b} \otimes \boldsymbol{\delta}(L)) \boldsymbol{\delta}(A_C) dV = \mathbf{b}, \quad (3.37)$$

where in the first equality the definition of surface generalized function (for  $A_C$ ) has been used. In writing (3.37)<sub>2</sub> we have implicitly assumed the orthogonality of  $L$  and  $A_C$  at their point of intersection, say  $\mathbf{X}_0$ . The final relation (3.37)<sub>3</sub> is then a direct consequence of (3.35). Using (3.34), it is easy to check that for  $\boldsymbol{\alpha}_r$  defined in (3.36)

$$\text{Div } \boldsymbol{\alpha}_r^T = \mathbf{0}. \quad (3.38)$$

We can similarly obtain a formula for  $\mathbf{K}^{-1}$ , which should be such that its integral over any material curve (say  $C$ ) which encloses the dislocation line  $L$ , must equal the constant  $\mathbf{b}$ . The following expression satisfies this requirement (cf. equation (27.8) in [96])

$$\mathbf{K}^{-1} = \mathbf{1} + (\mathbf{b} \otimes \boldsymbol{\delta}(S)), \quad (3.39)$$

where  $S$  is any surface bounded by  $L$ , such that it meets  $C$  orthogonally. This expression for  $\mathbf{K}^{-1}$  is compatible with that of  $\boldsymbol{\alpha}_r$  in (3.36), in the sense that  $\text{Curl } \mathbf{K}^{-1} = \boldsymbol{\alpha}_r$ . This follows at once from (3.33) and (2.20). Note that, unlike the representation (3.36), the expression for  $\mathbf{K}^{-1}$  is non-unique. This is due to the fact that there might be infinite number of surfaces  $S$  which are bounded by  $L$  and intersect  $C$  orthogonally. Any combination of expressions of the type (3.39) for each of these surfaces will give us a valid representation for  $\mathbf{K}^{-1}$  (with obvious adjustments for  $\mathbf{b}$ ).

### 3.2.3 Geometrically necessary and statistically stored dislocations

Recall that plastic distortion  $\mathbf{K}$  maps a local neighborhood in the relaxed configuration  $\kappa_i$  to a local neighborhood in the fixed reference configuration. The size of the local neighborhood (as implied from our discussion in Section 3.1) is such that every dislocation can be distinctly identified. Since otherwise, there would still remain a distribution of internal stresses, if only locally.<sup>8</sup> On the other hand, plastic distortion can be considered in an average sense, i.e. averaged over a representative volume element (RVE). A need for such averaging arises, for example, in cases where due to limitations of the experimental technique, measurements are restricted by the scale of the observation. Furthermore, in many problems, we are interested only in a macroscopic response. The classical theory of plasticity itself is a macroscopic theory, with the notion of plastic strain understood only in an average sense (cf. Chapter 2 in [4]).

As a result of averaging, each RVE has an associated plastic distortion. The distribution, over the body, of (averaged) dislocation density is then, a result of the incompatibility between different RVE's induced by an inhomogeneous (averaged) plastic distortion field, and is termed as *geometrically necessary dislocation density* (GND). Of course, as a result of averaging, much information about the microstructure is lost. To characterize this lost information, another measure called *statistically stored dislocation density* (SSD) is introduced. This name derives from the fact that SSD, unlike GND, is not geometric in nature, but is purely a consequence of random interactions among dislocations in the RVE [6]. Therefore, given a plastic distortion field in the body, one can obtain the resultant

---

<sup>8</sup>At this point, the term *local* has no scale attached to it. Exploiting the nature of the continuum, it can be arbitrarily small in diameter.

GND via a formula of the type (3.22)<sub>1</sub>. However, to obtain any information regarding SSD, one has to specify (or presume) additional information about the microstructure and the averaging method used. We emphasize that the concepts of GND and SSD are intrinsic to selecting a preferred (length) scale of plastic deformation in the theory and their nature depends not only on the *true* microstructure of the body, but also on the averaging method.

For example, if we consider the whole body as our RVE, the average plastic distortion field will be homogeneous and there would be no net GND, but there will be a non zero distribution of SSD. On the other hand, if we choose the dimensions of the RVE such that each individual dislocation is identifiable, then GND will be the total dislocation density and SSD would be zero. The notion of an average dislocation density was first introduced by Nye [134] who expressed the dislocation density in terms of the number of dislocation lines crossing a unit area (see also [90]). Later, Ashby [6]<sup>9</sup> provided a physical basis for GND and SSD and demonstrated their emergence in plastically inhomogeneous deformations. It was however, not until the paper by Arsenlis and Parks [5], that a precise distinction between GND and SSD was made. They considered a RVE (of volume  $V$ ) and obtained the associated average dislocation density (calling it Nye's tensor) as a line integral of all the dislocations within the RVE.

We will now use the distributions for single dislocations (from previous subsection) and present the ideas of Arsenlis and Parks [5] in a different light. Consider a simple volume average of type – “ $a$ ” of dislocations, with each dislocation line being treated as a separate

---

<sup>9</sup>The terms GND and SSD are coined in this paper.



entity, represented by the dislocation density as in (3.36). Define (cf. [92])

$$\bar{\alpha}_r = \frac{1}{V} \int_V \sum_{\xi=1}^a \alpha_r^{(\xi)} dV, \quad (3.40)$$

where

$$\alpha_r^{(\xi)} = \delta(L^{(\xi)}) \otimes \mathbf{b}^{(\xi)}. \quad (3.41)$$

Substituting this back into (3.40) we obtain

$$\bar{\alpha}_r = \frac{1}{V} \sum_{\xi=1}^a \int_{L^{(\xi)}} d\mathbf{L}^{(\xi)} \otimes \mathbf{b}^{(\xi)}. \quad (3.42)$$

Let  $\mathbf{r}^{(\xi)} = \int_{L^{(\xi)}} d\mathbf{L}^{(\xi)}$ ,  $\bar{l}^{(\xi)} = |\mathbf{r}^{(\xi)}|$ , and  $\bar{\mathbf{t}}^{(\xi)} = \frac{\mathbf{r}^{(\xi)}}{|\mathbf{r}^{(\xi)}|}$ . Equation (3.42) can then be written as (cf. equation (6) in [5])

$$\bar{\alpha}_r = \sum_{\xi=1}^a \rho_{GN}^{(\xi)} \bar{\mathbf{t}}^{(\xi)} \otimes \mathbf{b}^{(\xi)}, \quad (3.43)$$

where

$$\rho_{GN}^{(\xi)} = \frac{\bar{l}^{(\xi)}}{V} \quad (3.44)$$

is the geometric dislocation length (of dislocation  $\xi$ ) per unit volume of the representative volume element. It is of course different from the total dislocation line length, the difference being the statistical dislocation length. Similarly, define the volume average for the plastic distortion as

$$\bar{\mathbf{K}}^{-1} = \frac{1}{V} \int_V \sum_{\xi=1}^a \mathbf{K}^{-1(\xi)} dV, \quad (3.45)$$

where from (3.39)

$$\mathbf{K}^{-1(\xi)} = \mathbf{1} + (\mathbf{b}^{(\xi)} \otimes \delta(S^{(\xi)})). \quad (3.46)$$

If we restrict each of the  $\mathbf{K}^{-1(\xi)}$  to a specific plane,<sup>10</sup> with (fixed) unit normal  $\mathbf{N}^{(\xi)}$  and an

---

<sup>10</sup>Thus restricting slip to a few planes. In crystal plasticity, these planes are the crystallographic planes on which slip occurs.

area (inside the RVE)  $A^{(\xi)}$ , then equation (3.45) takes the form

$$\bar{\mathbf{K}}^{-1} = \mathbf{1} + \sum_{\xi=1}^a \gamma^{(\xi)} \mathbf{s}^{(\xi)} \otimes \mathbf{N}^{(\xi)}, \quad (3.47)$$

where

$$\gamma^{(\xi)} = \frac{A^{(\xi)}}{V} |\mathbf{b}^{(\xi)}|, \quad \text{and } \mathbf{s}^{(\xi)} = \frac{\mathbf{b}^{(\xi)}}{|\mathbf{b}^{(\xi)}|} \quad (3.48)$$

denote net plastic slip and the unit slip direction, respectively. The geometric line length  $\rho_{GN}^{(\xi)}$  can be written in terms of the gradients of  $\gamma^{(\xi)}$  as

$$\rho_{GN}^{(\xi)} = \sqrt{\left(\rho_{GN(e)}^{(\xi)}\right)^2 + \left(\rho_{GN(s)}^{(\xi)}\right)^2}, \quad (3.49)$$

where

$$\rho_{GN(e)}^{(\xi)} |\mathbf{b}^{(\xi)}| = -\nabla \gamma^{(\xi)} \cdot \mathbf{s}^{(\xi)}, \quad \text{and } \rho_{GN(s)}^{(\xi)} |\mathbf{b}^{(\xi)}| = \nabla \gamma^{(\xi)} \cdot \mathbf{m}^{(\xi)} \quad (3.50)$$

are the edge and the screw components of the geometric dislocation length, respectively. In (3.50)<sub>2</sub>,  $\mathbf{m}^{(\xi)} = \mathbf{s}^{(\xi)} \times \mathbf{N}^{(\xi)}$ . These results can be obtained on using (3.22)<sub>1</sub>, (3.47) and (3.43). The above illustration clearly demonstrates the relationship of macroscopic plastic distortion to local plastic distortion.

In constructing continuum plasticity theories, we usually consider (implicitly) the plastic distortion in a macroscopic sense. The resulting dislocation distribution is then GND. Additional parameters of state are therefore required to characterize SSD, whose importance in plastic flow had been demonstrated in many works [123]. We, however, will neglect any contributions from SSD in our constitutive relations, and thus identify GND with the net dislocation density field. In doing so, we are assuming that the role of dislocations in plastic flow is completely characterized by GND. For an implication of this assumption on hardening, see the first remark in Section 3.8.

### 3.3 Invariance under compatible changes in the reference configuration

Before we move on to a discussion on the thermodynamics of plastic flow, we state and prove a result of central importance in our formulation. This result is concerned with obtaining restrictions on constitutive equations due to their invariance with respect to *compatible* changes in the reference configuration. We call two configurations compatible, if their point spaces are related by a continuously differentiable map.

Any constitutive function should be invariant with respect to arbitrary changes in the reference configuration, unless it is defined explicitly with respect to a particular reference configuration.<sup>11</sup> This results from the fact that our selection of a reference configuration is purely a matter of convenience and the response of the body should be invariant to *our* choice of a reference configuration. However the reference configurations are restricted to be subsets of the Euclidean point space. Therefore they should be related only through a compatible mapping. In this section we will restrict our attention to constitutive functions defined away from the singular surface. The representation for functions defined on a singular surface will be obtained later in Chapter 6.

Let us denote a (time independent) compatible change in the reference configuration  $\kappa_{r_1}$  by a smooth and invertible mapping  $\boldsymbol{\lambda} : \kappa_{r_1} \rightarrow \kappa_{r_2}$ , where  $\kappa_{r_2}$  denotes the new reference configuration (cf. the discussion following (3.23)). Therefore  $\mathbf{X}_2 = \boldsymbol{\lambda}(\mathbf{X}_1)$  where

---

<sup>11</sup>An example of this is furnished by the standard form of the strain energy density in the classical theories of elasticity, i.e.  $W(\mathbf{F})$ . This strain energy represents the material response for distortions with respect to a reference configuration.

$\mathbf{X}_1 \in \kappa_{r_1}$  and  $\mathbf{X}_2 \in \kappa_{r_2}$ . Let the gradient associated with this mapping be  $\mathbf{A} = \nabla_1 \boldsymbol{\lambda}$ . Here  $\nabla_1$  and  $\nabla_2$  represent the gradient with respect to  $\mathbf{X}_1$  and  $\mathbf{X}_2$ , respectively. The intermediate and the current configurations are invariant under such a transformation. It is then straightforward to obtain the following:

$$\mathbf{K}_2 = \mathbf{A}\mathbf{K}_1, \quad \mathbf{H}_2 = \mathbf{H}_1, \quad \text{and} \quad \mathbf{F}_2 = \mathbf{F}_1\mathbf{A}^{-1} \quad (3.51)$$

A scalar function<sup>12</sup>  $\Psi = \hat{\Psi}(\mathbf{H}_1, \mathbf{K}_1^{-1}, \dot{\mathbf{H}}_1, \dot{\mathbf{K}}_1^{-1}, \nabla_1 \mathbf{K}_1^{-1}, \theta_1, \mathbf{g}_1)$ , where  $\mathbf{g}_1 = \nabla_1 \theta_1$  and  $\dot{\mathbf{K}}_1^{-1}$  denotes the time derivative of  $\mathbf{K}^{-1}$ , is invariant under the change in reference configuration to  $\kappa_{r_2}$  if

$$\hat{\Psi}(\mathbf{H}_1, \mathbf{K}_1^{-1}, \dot{\mathbf{H}}_1, \dot{\mathbf{K}}_1^{-1}, \nabla_1 \mathbf{K}_1^{-1}, \theta_1, \mathbf{g}_1) = \hat{\Psi}(\mathbf{H}_2, \mathbf{K}_2^{-1}, \dot{\mathbf{H}}_2, \dot{\mathbf{K}}_2^{-1}, \nabla_2 \mathbf{K}_2^{-1}, \theta_2, \mathbf{g}_2). \quad (3.52)$$

The choice of arguments for the function  $\Psi$  is motivated partially by our discussion on the thermodynamics of plastic flow (see next section), where we assume  $\{\mathbf{F}, \mathbf{H}, \theta\}$  to be the set of state variables. In the set of state variables,  $\mathbf{F}$  can be replaced by  $\mathbf{H}\mathbf{K}^{-1}$  (cf. (3.18)). The inclusion of rate terms and the temperature gradient term  $\mathbf{g}$  is motivated from the dissipation inequality (3.75) (we can also include  $\dot{\theta}$  in the list of arguments, without any loss of generality). The term  $\nabla_1 \mathbf{K}^{-1}$  is included since, as we shall see below, the dependence of  $\Psi$  on  $\mathbf{K}^{-1}$  (in an isothermal case) can only be through a rate term of the form  $\mathbf{K}^{-1}\dot{\mathbf{K}}$  or through  $\boldsymbol{\alpha}$ . If  $\nabla_1 \mathbf{K}^{-1}$  would have been excluded from the list of variables, the dependence would have been only through  $\mathbf{K}^{-1}\dot{\mathbf{K}}$ . This would in turn imply that the flow rule for the evolution of plastic distortion (see Section 3.7) would be independent of  $\mathbf{K}$  (or its gradient)

---

<sup>12</sup>Similar considerations apply to vector and tensor valued functions, which belong to the intermediate configuration, i.e. vectors and tensors defined as, say,  $\mathbf{c} \in \kappa_i$  and  $\mathbf{C} : \kappa_i \rightarrow \kappa_i$ , respectively.

and therefore would fail to capture effects such as hardening which depend on the state of plasticity in the body.

It follows from (3.51)<sub>1,2</sub> and  $\dot{\boldsymbol{\lambda}} = \mathbf{0}$  that

$$\dot{\mathbf{K}}_2^{-1} = \dot{\mathbf{K}}_1^{-1} \mathbf{A}^{-1} \quad \text{and} \quad \dot{\mathbf{H}}_2 = \dot{\mathbf{H}}_1. \quad (3.53)$$

To relate the gradients, use  $d\mathbf{K}_2^{-1} = (\nabla_2 \mathbf{K}_2^{-1}) d\mathbf{X}_2 = (\nabla_2 \mathbf{K}_2^{-1}) \mathbf{A} d\mathbf{X}_1$  to obtain

$$\nabla_2 \mathbf{K}_2^{-1} = (\nabla_1 \mathbf{K}_2^{-1}) \mathbf{A}^{-1}. \quad (3.54)$$

Expressing this in terms of components we write,

$$\begin{aligned} (\nabla_2 \mathbf{K}_2^{-1})_{ijl} &= A_{kl}^{-1} K_{2ij,k}^{-1} \\ &= A_{kl}^{-1} A_{mj}^{-1} K_{1im,k}^{-1} + A_{kl}^{-1} A_{mj,k}^{-1} K_{1im}^{-1}, \end{aligned} \quad (3.55)$$

where in (3.55)<sub>2</sub> the relation  $\mathbf{K}_2^{-1} = \mathbf{K}_1^{-1} \mathbf{A}^{-1}$  has been used. Furthermore

$$\theta_2 = \theta_1, \quad \text{and} \quad \mathbf{g}_2 = \mathbf{g}_1 \mathbf{A}^{-1}, \quad (3.56)$$

where to obtain (3.56)<sub>2</sub> use  $d\theta = \nabla_2 \theta d\mathbf{X}_2 = \nabla_1 \theta d\mathbf{X}_1$  and  $d\mathbf{X}_2 = \mathbf{A} d\mathbf{X}_1$ .

To obtain a necessary condition choose  $\mathbf{A}^{-1}$  such that  $A_{kl}^{-1}(\mathbf{X}_0) = \delta_{kl}$  but with  $\nabla_1 \mathbf{A}^{-1}(\mathbf{X}_0) \neq \mathbf{0}$ , where  $\mathbf{X}_0 \in \kappa_{r_1}$  is the point at which equation (3.52) is evaluated. Use this choice of  $\mathbf{A}$  in (3.51)<sub>1,2</sub>, (3.53), (3.55)<sub>2</sub>, and (3.56) and consequently obtain from (3.52)

$$\hat{\Psi}(\mathbf{H}_1, \mathbf{K}_1^{-1}, \dot{\mathbf{H}}_1, \dot{\mathbf{K}}_1^{-1}, \nabla_1 \mathbf{K}_1^{-1}, \theta_1, \mathbf{g}_1) = \hat{\Psi}(\mathbf{H}_1, \mathbf{K}_1^{-1}, \dot{\mathbf{H}}_1, \dot{\mathbf{K}}_1^{-1}, \nabla_1 \mathbf{K}_1^{-1} + \mathbf{K}_1^{-1} \nabla_1 \mathbf{A}^{-1}, \theta_1, \mathbf{g}_1) \quad (3.57)$$

at some  $\mathbf{X}_0 \in \kappa_{r_1}$ . Furthermore, obtain from (3.55)<sub>2</sub> (at  $\mathbf{X}_0$ )

$$Sym_{jl}(\nabla_2 \mathbf{K}_2^{-1})_{ijl}(\mathbf{X}_0) = Sym_{jl}(K_{1ij,l}^{-1}) + A_{mj,l}^{-1} P_{1im}^{-1}, \quad (3.58)$$

where  $Sym_{jl} B_{ijl} = \frac{1}{2}(B_{ijl} + B_{ilj})$  for some arbitrary third order tensor  $\mathbf{B}$ . In obtaining (3.58), we have also made use of the fact that  $A_{ml}^{-1}$  is a gradient. The skew part, on the other hand is given by (at  $\mathbf{X}_0$ )

$$Skw_{jl}(\nabla_2 \mathbf{K}_2^{-1})_{ijl} = Skw_{jl}(K_{1ij,l}^{-1}), \quad (3.59)$$

where  $Skw_{jl} B_{ijl} = \frac{1}{2}(B_{ijl} - B_{ilj})$ . Therefore, the symmetric part  $Sym_{jl}(\nabla_2 \mathbf{K}_2^{-1})_{ijl}$  is the only term, among all the arguments of function  $\Psi$ , which depends on the transformation mapping. Consequently it can be changed while other arguments are kept fixed. Therefore  $\Psi$  cannot depend on this term. Equation (3.57) then reduces to

$$\hat{\Psi}(\mathbf{H}_1, \mathbf{K}_1^{-1}, \dot{\mathbf{H}}_1, \mathbf{K}_1^{-1}, \nabla_1 \mathbf{K}_1^{-1}, \theta_1, \mathbf{g}_1) = \tilde{\Psi}(\mathbf{H}_1, \mathbf{K}_1^{-1}, \dot{\mathbf{H}}_1, \mathbf{K}_1^{-1}, K_{1ij,l}^{-1} - K_{1il,j}^{-1}, \theta_1, \mathbf{g}_1) \quad (3.60)$$

Consider two arbitrary constant vectors  $\mathbf{a} \in \mathcal{V}$  and  $\mathbf{b} \in \kappa_i$ . Define another vector  $\mathbf{p} \in \mathcal{V}$  by  $\mathbf{p} = \mathbf{K}_1^{-T} \mathbf{b}$ . Therefore

$$(\nabla_1 \mathbf{p})_{jl} = K_{1ij,l}^{-1} b_i \quad \text{and} \quad 2Skw(\nabla_1 \mathbf{p})_{jl} = (K_{1ij,l}^{-1} - K_{1il,j}^{-1}) b_i \quad (3.61)$$

As a result

$$(K_{1ij,l}^{-1} - K_{1il,j}^{-1}) b_i a_l = (2Skw(\nabla_1 \mathbf{p}) \mathbf{a})_j = (\text{Curl}(\mathbf{p}) \times \mathbf{a})_j = (\text{Curl}(\mathbf{K}_1^{-1}) \mathbf{b} \times \mathbf{a})_j, \quad (3.62)$$

where the first equality derives from (3.61)<sub>2</sub>. The second equality is an identity and can be verified by expressing all the terms in indicial notation. The third equality is a consequence of the definition of Curl operator (cf. (2.20)). The outer equality in (3.62) then implies that we can replace the term  $(K_{1ij,l}^{-1} - K_{1il,j}^{-1})$  in (3.60) by  $\text{Curl}(\mathbf{K}_1^{-1})$ . Therefore, a *necessary* condition for  $\Psi$  to be invariant is

$$\Psi = \tilde{\Psi}(\mathbf{H}_1, \mathbf{K}_1^{-1}, \dot{\mathbf{H}}_1, \mathbf{K}_1^{-1}, \text{Curl}(\mathbf{K}_1^{-1}), \theta_1, \mathbf{g}_1). \quad (3.63)$$

Next, consider  $\mathbf{A}^{-1}$  such that it is homogeneous and equal to the local value of  $\mathbf{K}_1$ . That is  $\mathbf{A}^{-1}(\mathbf{X}) = \mathbf{K}_1(\mathbf{X}_0)$ , for all  $\mathbf{X} \in \kappa_r$  and some  $\mathbf{X}_0 \in \kappa_r$ . Under such a transformation, therefore (at  $\mathbf{X}_0$ )

$$\mathbf{K}_2^{-1} = \mathbf{1}, \quad \dot{\mathbf{K}}_2^{-1} = \dot{\mathbf{K}}_1^{-1} \mathbf{K}_1, \quad \text{Curl}_2(\mathbf{K}_2^{-1}) = J_{K_1} \mathbf{K}_1^{-1} \text{Curl}_1(\mathbf{K}_1^{-1}), \quad \text{and } \mathbf{g}_2 = \mathbf{g}_1 \mathbf{K}_1, \quad (3.64)$$

where (3.64)<sub>1,2</sub> follows from (3.51)<sub>1</sub> and (3.53)<sub>1</sub>, respectively, and (3.64)<sub>3</sub> has been proved earlier in (3.26). The relation (3.64)<sub>4</sub> follows from (3.56)<sub>2</sub>. Therefore, if  $\Psi$  is invariant under compatible changes in the reference configuration, it takes the following form

$$\Psi = \check{\Psi}(\mathbf{H}, \dot{\mathbf{H}}, \mathbf{K}^{-1} \mathbf{K}, J_K \mathbf{K}^{-1} \text{Curl}(\mathbf{K}^{-1}), \theta, \mathbf{g} \mathbf{K}). \quad (3.65)$$

It is straightforward to check that such a form of  $\Psi$  is also *sufficient* for it to be invariant under compatible changes in the reference configuration. This can be done by directly substituting (3.51)<sub>1,2</sub> in (3.65). Thus, representation (3.65) furnishes us with a necessary and sufficient condition for  $\Psi$  to be invariant under compatible changes in the reference configuration. A similar result has been obtained earlier by Cermelli and Gurtin [30] in the context of continuum plasticity, and by Davini, Parry and Šilhavý [42, 139, 138] in the context of a formulation based on crystal lattice vectors.

A most important conclusion, as implied from (3.65), is that  $\Psi$  can be a function of  $\mathbf{K}^{-1}$  and  $\nabla \mathbf{K}^{-1}$  only through a dependence on the rate term<sup>13</sup>  $\mathbf{K}^{-1} \dot{\mathbf{K}}$ , the true dislocation density tensor  $\boldsymbol{\alpha}$  or through the temperature gradient term  $\mathbf{g} \mathbf{K}$ .

---

<sup>13</sup>The rate term can be rewritten using  $\mathbf{K} \mathbf{K}^{-1} = \mathbf{1}$ , as  $\mathbf{K}^{-1} \dot{\mathbf{K}} = -\mathbf{K}^{-1} \dot{\mathbf{K}}$ , where we note again that  $\dot{\mathbf{K}}^{-1}$  denotes the time derivative of  $\mathbf{K}^{-1}$  and is therefore not same as  $\dot{\mathbf{K}}^{-1}$ , which is the inverse of the time derivative of  $\mathbf{K}$ .

## 3.4 Thermodynamics of plastic flow

In this section, We recall our discussion on the second law of thermodynamics from Subsection 2.2.3, and make further assumptions on the nature of state variables and constitutive functions. Restrictions on the plastic evolution are then obtained at points away from the singular surface and on the singular surface. After this chapter, we will limit our attention to isothermal and adiabatic processes only, and therefore we provide in a subsection below, the form of governing equations for these processes.

### 3.4.1 State variables and constitutive assumptions

The thermodynamical state of each material neighborhood is assumed to be determined completely by  $\mathbf{F}$ ,  $\mathbf{H}$ , and  $\theta$ . We right away make a distinction between *controllable* variables and *uncontrollable* ones. The absolute temperature can of course be controlled (at least in principle) by using temperature baths. A mechanical variable, on the other hand, is controllable if it can be coupled to an external *force* field which can control its value [18]. The mechanical work, therefore, can be written only for controllable variables. A variable is *observable* if its value can be experimentally determined, a property which is essential for it to qualify as a state variable. The deformation map  $\mathbf{F}$  can be both observed and controlled while the elastic distortion  $\mathbf{H}$  can only be observed but not controlled [21, 85]. The controllability of  $\mathbf{F}$  stems from the fact that it appears as a result of the local gradient of the spatial position at a fixed material point. The spatial position, as our experiences show, can be controlled via a force. Regarding the observability of  $\mathbf{F}$ , it can be obtained by tracking the deformation map  $\chi$  for each neighborhood of the body. The elastic dis-



tortion  $\mathbf{H}$ , however, is related to the local distortion of a neighborhood. For crystals it represents the local distortion of lattice vectors. In the absence of dislocations, it retains the character of  $\mathbf{F}$  and a distinction is then superfluous. But otherwise, it also measures the local dislocation content at a material point. The reason that it is *not* controllable, comes from the fact that there does not exist an independent forcing mechanism by which we can control its value. In recent years there have been successful advancements in observing  $\mathbf{H}$ . One such technique for crystals is to use X-ray microscopy in which lattice distortions are measured with respect to an unstressed crystal configuration [100, 113]. These techniques are, however, still restricted to small elastic distortions.

Note that since  $\mathbf{H}$  and  $\nabla\mathbf{H}$  (hence  $\boldsymbol{\alpha}$ ) are independent at a material point, we could have included dislocation density  $\boldsymbol{\alpha}$  as an independent state variable. However, we simply assume that  $\mathbf{H}$  alone affects the state of the lattice while  $\boldsymbol{\alpha}$  affects its yield (see Section 3.7).

Also, contrary to most of the treatments on plasticity, we do not restrict our attention to isochoric plastic flow. Therefore  $J_K = \det \mathbf{K} \neq 1$ . Such a restriction has been found to be unnecessary in many experiments [19, 11].

**Constitutive assumptions** A constitutive function is a scalar, vector or tensor valued function, which contains information about the response of the system at hand. A distinction should, however, be made between constitutive functions which are functions of the state, i.e. dependent only on the state variables, and those which can depend on state variables and also on their temporal and spatial gradients. It is functions of the latter kind, which are used to characterize an irreversible behavior. Possible examples of the functions

of state are specific energy and specific entropy. Examples of constitutive functions dependent also on the gradients of state variables are furnished by the yield surface and the plastic flow rule (see Section 3.7). Further, we assume that we are dealing with materially uniform bodies (cf. Remark 3.8.3), and thus there is no explicit dependence on  $\mathbf{X}$  in any of the constitutive functions.

These constitutive functions should follow the invariance requirements mentioned in Section 3.3. Let us denote by  $W$ , the free energy density per unit volume of the intermediate configuration. It is a state function, and therefore a function of  $\mathbf{F}$ ,  $\mathbf{H}$ , and  $\theta$ . But the invariance requirement imposed in Section 3.3 restricts it to have the following form

$$W = \hat{W}(\mathbf{H}, \theta). \quad (3.66)$$

This function describes the response of the material to distortion induced by the map from  $\kappa_i$  to  $\mathcal{V}$  at  $\mathbf{x} \in \kappa_t$ . The specific free energy with respect to the reference configuration is given by  $\rho_\kappa f = J_K^{-1} \hat{W}(\mathbf{H}, \theta)$ . Similarly, specific entropy  $\eta$  with respect to the reference configuration can be expressed as  $\rho_\kappa \eta = J_K^{-1} S$ , where  $S = \hat{S}(\mathbf{H}, \theta)$  is the total entropy per unit volume of the intermediate configuration.

Under the hypothesis that stress is purely elastic in origin, we assume the Cauchy stress  $\mathbf{T} \in Sym$  and the entropy  $S$  to be given by

$$J_H \mathbf{T} = W_{\mathbf{H}} \mathbf{H}^T, \quad \text{and } S = -W_\theta. \quad (3.67)$$

The Piola stress is related to Cauchy stress by  $\mathbf{P} = \mathbf{T} \mathbf{F}^*$  and therefore we can obtain

$$\mathbf{P} \mathbf{K}^* = W_{\mathbf{H}}. \quad (3.68)$$

### 3.4.2 Dissipation

Recall the local form of the Clausius-Duhem inequality from Chapter 2 (cf. (2.198) and (2.204))

$$\rho_\kappa \dot{f} - \mathbf{P} \cdot \dot{\mathbf{F}} + \rho_\kappa \eta \dot{\theta} + \frac{\mathbf{q} \cdot \mathbf{g}}{\theta} \leq 0, \quad (3.69)$$

outside the singular surface and

$$U \left( \mathbf{N}_s \cdot \llbracket \mathbf{E} \rrbracket \mathbf{N}_s + \frac{1}{2} U^2 \rho_\kappa \llbracket |\mathbf{F} \mathbf{N}_s|^2 \rrbracket \right) + \left( U \rho_\kappa \langle \eta \rangle - \left\langle \frac{\mathbf{q}}{\theta} \right\rangle \cdot \mathbf{N}_s \right) \llbracket \theta \rrbracket \geq 0 \quad (3.70)$$

at the singular surface  $S_t$ , where  $\mathbf{E} = \rho_\kappa f \mathbf{1} - \mathbf{F}^T \mathbf{P}$  is the Eshelby tensor. We now simplify these relations using our constitutive assumptions.

Use (3.66), (3.68), and (3.67)<sub>2</sub> to write

$$\dot{W} = \mathbf{P} \mathbf{K}^* \cdot \dot{\mathbf{H}} - S \dot{\theta}. \quad (3.71)$$

Substitute this in

$$\rho_\kappa \dot{f} = J_K^{-1} \dot{W} - J_K^{-2} J_K \dot{W} \quad (3.72)$$

and use  $\dot{J}_K = J_K \mathbf{K}^{-T} \cdot \dot{\mathbf{K}}$  to obtain

$$\rho_\kappa \dot{f} = \mathbf{P} \cdot \dot{\mathbf{F}} + (\mathbf{F}^T \mathbf{P} - J_K^{-1} W \mathbf{1}) \mathbf{K}^{-T} \cdot \dot{\mathbf{K}} - J_K^{-1} S \dot{\theta}, \quad (3.73)$$

where we have also used the relation

$$\dot{\mathbf{H}} = \dot{\mathbf{F}} \mathbf{K} + \mathbf{F} \dot{\mathbf{K}}, \quad (3.74)$$

which follows from (3.18). Substitute (3.73) in (3.69) to get [47]

$$D \equiv \mathbf{E} \cdot \dot{\mathbf{K}} \mathbf{K}^{-1} - \frac{\mathbf{q} \cdot \mathbf{g}}{\theta} \geq 0, \quad (3.75)$$

with  $D$  denoting the dissipation (or rate of internal entropy generation, cf. (2.186)), per unit volume of the reference configuration. Further, using (3.68) and (3.18), Eshelby's tensor may be written in the form

$$\mathbf{E} = J_K^{-1} \mathbf{K}^{-T} \mathbf{E}' \mathbf{K}^T, \quad (3.76)$$

where

$$\mathbf{E}' = W \mathbf{1} - \mathbf{H}^T W_{\mathbf{H}} \quad (3.77)$$

is purely elastic in origin. This in turn yields

$$D = J_K^{-1} \mathbf{E}' \cdot \mathbf{K}^{-1} \dot{\mathbf{K}} - \frac{\mathbf{q} \cdot \mathbf{g}}{\theta}. \quad (3.78)$$

Consequently, dissipation away from the surface  $S_t$  vanishes if

$$\dot{\mathbf{K}} = \mathbf{0}, \quad \text{and} \quad \mathbf{g} = \mathbf{0} \quad (3.79)$$

or if

$$J_K^{-1} \mathbf{E}' \cdot \mathbf{K}^{-1} \dot{\mathbf{K}} = \frac{\mathbf{q} \cdot \mathbf{g}}{\theta}. \quad (3.80)$$

Therefore in addition to (3.79), where there is no plastic and heat flow, (3.80) represents a condition under which the production of entropy via plasticity is compensated with that produced via heat flow, so as to avoid irreversibility, if only locally. Processes as governed by (3.75) are *thermodynamically coupled*<sup>14</sup> in a sense that the evolution of one dissipative process (plasticity) is coupled with the other (heat conduction). Such a coupling allows for a process (here, plastic flow or heat conduction) to evolve in a direction contrary to the one

---

<sup>14</sup>See Prigogine [146, 57] for more on the notion of *coupling* in similar contexts. An illustrative example is provided by Bénard instability in hydrodynamics ([57], Chapter 11). There, a relation similar to (3.80) (with viscosity instead of plasticity) provides a criterion for the onset of instability.

prescribed, when the processes exist independently. Therefore, the nature of plastic flow can be significantly different in the presence of heat conduction compared to the situation when heat conduction is neglected (for example, isothermal and adiabatic processes). With this in mind, we will, however, restrict our discussions only to isothermal and adiabatic processes (see the following subsection).

To clarify the contribution of plastic flow on the surface, we use (3.76) and (2.46) to write the jump in  $\mathbf{E}$  as

$$\begin{aligned} \llbracket \mathbf{E} \rrbracket &= \llbracket \mathbf{K}^{-T} \rrbracket \langle J_K^{-1} \mathbf{E}' \mathbf{K}^T \rangle + \langle \mathbf{K}^{-T} \rangle \llbracket J_K^{-1} \mathbf{E}' \mathbf{K}^T \rrbracket \\ &= \llbracket \mathbf{K}^{-T} \rrbracket \langle J_K^{-1} \mathbf{E}' \mathbf{K}^T \rangle + \langle \mathbf{K}^{-T} \rangle \langle \mathbf{E}' \rrbracket \llbracket J_K^{-1} \mathbf{K}^T \rrbracket + \langle \mathbf{K}^{-T} \rangle \llbracket \mathbf{E}' \rrbracket \langle J_K^{-1} \mathbf{K}^T \rangle. \end{aligned} \quad (3.81)$$

Also, use (3.18) and (2.46) to write

$$\frac{1}{2} \llbracket \mathbf{F} \mathbf{N}_s \cdot \mathbf{F} \mathbf{N}_s \rrbracket = \llbracket \mathbf{K}^{-1} \rrbracket \mathbf{N}_s \cdot \langle \mathbf{H}^T \rangle \langle \mathbf{F} \mathbf{N}_s \rangle + \langle \mathbf{K}^{-1} \rangle \mathbf{N}_s \cdot \llbracket \mathbf{H}^T \rrbracket \langle \mathbf{F} \mathbf{N}_s \rangle. \quad (3.82)$$

Substitute (3.81)<sub>2</sub> and (3.82) into (3.70) to obtain

$$\begin{aligned} & U \mathbf{N}_s \cdot (\llbracket \mathbf{K}^{-T} \rrbracket \langle J_K^{-1} \mathbf{E}' \mathbf{K}^T \rangle + \langle \mathbf{K}^{-T} \rangle \langle \mathbf{E}' \rrbracket \llbracket J_K^{-1} \mathbf{K}^T \rrbracket + U^2 \rho_\kappa \llbracket \mathbf{K}^{-T} \rrbracket \langle \mathbf{H}^T \rangle \langle \mathbf{F} \rangle) \mathbf{N}_s \\ & + \left\{ U \mathbf{N}_s \cdot (\langle \mathbf{K}^{-T} \rangle \llbracket \mathbf{E}' \rrbracket \langle J_K^{-1} \mathbf{K}^T \rangle + U^2 \rho_\kappa \langle \mathbf{K}^{-T} \rangle \llbracket \mathbf{H}^T \rrbracket \langle \mathbf{F} \rangle) \mathbf{N}_s \right. \\ & \left. + \left( U \rho_\kappa \langle \eta \rangle - \left\langle \frac{\mathbf{q}}{\theta} \right\rangle \cdot \mathbf{N}_s \right) \llbracket \theta \rrbracket \right\} \geq 0. \end{aligned} \quad (3.83)$$

In (3.83), we have divided in three lines, terms which are depend on  $\llbracket \mathbf{K} \rrbracket$ ,  $\llbracket \mathbf{H} \rrbracket$ , and  $\llbracket \theta \rrbracket$ , respectively. If we identify  $U \llbracket \mathbf{K} \rrbracket$  with the plastic flow at the surface, then the terms in the first line of (3.83) represent the contribution to the dissipation (at surface  $S_t$ ) due to plastic flow. The term inside  $\{\cdot\}$  then represents the usual production of surface dissipation in thermo-elasticity (cf. equation (3.7.10) in [156]).

*Remark 3.4.1.* (Vanishing plastic flow) There is no plastic flow in the body if  $\dot{\mathbf{K}} = \mathbf{0}$  away from  $S_t$  and  $U[\mathbf{K}] = \mathbf{0}$  on  $S_t$ . These conditions are equivalent to postulating that

$$\frac{d}{dt} \int_{\Omega} \mathbf{K} dV = \mathbf{0} \quad (3.84)$$

for all  $\Omega \subset \kappa_r$  such that  $\Omega \cap S_t \neq \emptyset$ . The validity of this proposition can be verified by invoking the transport theorem (2.113) and then using the localization theorem.

### 3.4.3 Isothermal and adiabatic processes

**Isothermal process** A process is isothermal if temperature  $\theta$  remains constant. Therefore  $\dot{\theta} = 0$ ,  $\mathbf{g} = \nabla\theta = \mathbf{0}$ , and  $[\theta] = 0$ . The free energy is given by  $\rho_{\kappa}f = J_K^{-1}\hat{W}(\mathbf{H})$ , and the Clausius-Duhem inequality reduces to

$$\mathbf{E} \cdot \dot{\mathbf{K}}\mathbf{K}^{-1} \geq 0, \quad (3.85)$$

outside the singular surface and

$$U \left( \mathbf{N}_s \cdot [\mathbf{E}]\mathbf{N}_s + \frac{1}{2}U^2\rho_{\kappa}[[\mathbf{F}\mathbf{N}_s|^2]] \right) \geq 0 \quad (3.86)$$

on the singular surface  $S_t$ . It is obvious from (3.85) that dissipation (away from  $S_t$ ) vanishes if  $\dot{\mathbf{K}}$  vanishes. To enforce the idea that plasticity is *inherently dissipative*, we adopt the following hypothesis:

$$\mathbf{E} \cdot \dot{\mathbf{K}}\mathbf{K}^{-1} > 0 \text{ if and only if } \dot{\mathbf{K}} \neq \mathbf{0}. \quad (3.87)$$

*In most of this thesis, we will assume processes to be isothermal.* An exception will be Chapter 5, which deals with plastic waves, where we will assume processes to be adiabatic.

**Adiabatic process** A process is adiabatic if heat flux  $\mathbf{q} = \mathbf{0}$  for all durations of time.

The equations for balance of energy, from (2.168) and (2.170), are reduced to

$$\rho_\kappa \dot{e} = \tilde{\mathbf{P}} \cdot \dot{\mathbf{F}} + \rho_\kappa r, \quad (3.88)$$

where  $\tilde{\mathbf{P}}$  is the adiabatic Piola stress, and

$$U \rho_\kappa [e] = U \langle \tilde{\mathbf{P}} \rangle \cdot \llbracket \mathbf{F} \rrbracket \quad (3.89)$$

outside and on the surface, respectively. The following constitutive assumptions are made

$$\rho_\kappa e = J_K^{-1} \tilde{W}(\mathbf{H}, \eta), \quad \theta = \tilde{\theta}(\mathbf{H}, \eta) \quad (3.90)$$

and

$$J_H \tilde{\mathbf{T}} = \tilde{W}_{\mathbf{H}} \mathbf{H}^T, \quad \rho_\kappa \theta = J_K^{-1} \tilde{W}_\eta, \quad (3.91)$$

where  $\tilde{\mathbf{T}}$  represents the adiabatic Cauchy stress. The adiabatic Piola stress is given by

$\tilde{\mathbf{P}} \mathbf{K}^* = \tilde{W}_{\mathbf{H}}$ . Using these constitutive assumptions, it is then not difficult to obtain

$$\rho_\kappa \dot{e} = \tilde{\mathbf{P}} \cdot \dot{\mathbf{F}} - J_K^{-1} \tilde{\mathbf{E}}' \cdot \mathbf{K}^{-1} \dot{\mathbf{K}} + \rho_\kappa \theta \dot{\eta}, \quad (3.92)$$

where

$$\tilde{\mathbf{E}}' = \tilde{W}_{\mathbf{1}} \mathbf{1} - \mathbf{H}^T \tilde{W}_{\mathbf{H}} \quad (3.93)$$

is the adiabatic Eshelby tensor. Substitute (3.92) into the balance of energy (3.88) to get

$$\rho_\kappa \theta \dot{\eta} = J_K^{-1} \tilde{\mathbf{E}}' \cdot \mathbf{K}^{-1} \dot{\mathbf{K}} + \rho_\kappa r, \quad (3.94)$$

which for vanishing body heat supply,  $r = 0$ , reduces to

$$\rho_\kappa \theta \dot{\eta} = J_K^{-1} \tilde{\mathbf{E}}' \cdot \mathbf{K}^{-1} \dot{\mathbf{K}}. \quad (3.95)$$

Use (3.94) into the Clausius-Duhem inequality (2.188) to get

$$J_K^{-1} \tilde{\mathbf{E}}' \cdot \mathbf{K}^{-1} \dot{\mathbf{K}} \geq 0. \quad (3.96)$$

On the surface, the dissipation inequality, as derived from (2.189), has the form

$$-U\rho_\kappa \llbracket \eta \rrbracket \geq 0. \quad (3.97)$$

We will come back to adiabatic approximation in Chapter 5, when we discuss plastic waves.

### 3.5 Superposed rigid motions<sup>15</sup>

Granted the symmetry of the Cauchy stress (cf. (2.157)), (3.67)<sub>1</sub> implies that

$$W_{\mathbf{H}} \cdot \mathbf{W}\mathbf{H} = \mathbf{0} \quad (3.98)$$

for any fixed  $\mathbf{W} \in Skw$ . Consider a parameterized path  $\mathbf{H}(u)$  defined by  $\dot{\mathbf{H}}(u) = \mathbf{W}\mathbf{H}$  with  $\mathbf{H}(0) = \mathbf{H}_0$ . The unique solution [67] is  $\mathbf{H}(u) = \mathbf{Q}(u)\mathbf{H}_0$ , where  $\mathbf{Q} \in Orth^+$  is a rotation with  $\mathbf{Q}(0) = \mathbf{1}$  and  $\dot{\mathbf{Q}}\mathbf{Q}^T = \mathbf{W}$ . This means that  $\dot{W} = 0$  on the path in question; i.e., that  $W(\mathbf{Q}\mathbf{H}_0) = W(\mathbf{H}_0)$  for any rotation  $\mathbf{Q}$ . Standard arguments based on Cauchy's theorem for hemitropic functions [170] or on the polar decomposition theorem then furnish (with the subscript <sub>0</sub> suppressed)

$$W(\mathbf{H}) = \hat{W}(\mathbf{C}_H) \quad \text{where} \quad \mathbf{C}_H = \mathbf{H}^T\mathbf{H}, \quad (3.99)$$

and thus

$$J_H \mathbf{T} = \mathbf{H}\mathbf{S}(\mathbf{C}_H)\mathbf{H}^T, \quad (3.100)$$

---

<sup>15</sup>Isothermal response will be assumed in the next two sections, without loss of any generality.



where

$$\mathbf{S}(\mathbf{C}_H) = 2\mathit{Sym}\hat{W}_{\mathbf{C}_H}. \quad (3.101)$$

Henceforth we assume that all constitutive hypotheses introduced in Section 3.1 apply to the function  $\hat{W}(\mathbf{C}_H)$ .

Note that in the course of deriving (3.100) we have assumed only the symmetry of the Cauchy stress. In particular, we have not imposed the invariance of the strain-energy function under superposed rigid-body motions. Indeed, in conventional finite elasticity theory, it is well known that invariance of the strain-energy function under superposed rigid-body motions is equivalent to symmetry of the Cauchy stress [170].

This issue leads us to consider the transformation rules for the elastic and plastic deformations under superposed rigid-body motions. In a way, this question is rendered meaningless if we understand  $\mathcal{M}$  to be a material manifold. For,  $\mathcal{M}$  is then indifferent to the placement of its points in  $\mathcal{E}$  and the issue of invariance under changes of such placements does not arise [130]. The fact that  $\mathbf{K}^{-1}$  maps  $\mathcal{V}$ , at  $\mathbf{X} \in \kappa_r$ , to  $T_{\mathcal{M}(p)}$ , at  $p = \kappa_i(X)$ , would then lead naturally to the conclusion that  $\mathbf{K}$  is invariant under superposed rigid-body motions. This would then dictate, via (3.18), the transformation rule  $\mathbf{H} \rightarrow \mathbf{QH}$ , where  $\mathbf{Q}(t)$  is the spatially uniform rotation in the conventional rule  $\mathbf{F} \rightarrow \mathbf{QF}$ . This is tacitly assumed in most works concerned with the invariance issue (e.g. [168, 30, 115, 125, 109]).

However, we can proceed in a different manner that emphasizes the constitutive character of the constituent elastic and plastic deformations. We know from conventional theory that

$$\mathbf{F} \rightarrow \mathbf{QF} \quad (3.102)$$

in a superposed rigid-body motion, where  $\mathbf{Q} \in Orth^+$ . This follows from the fact that  $\mathbf{x} \rightarrow \mathbf{Q}\mathbf{x} + \mathbf{c}$  in such a motion, with  $\mathbf{x} = \boldsymbol{\chi}(\mathbf{X}, t)$  and  $\mathbf{c}$  a function of  $t$  alone. We also assume that

$$\mathbf{T} \rightarrow \mathbf{Q}\mathbf{T}\mathbf{Q}^T, \quad \text{and therefore} \quad \mathbf{P} \rightarrow \mathbf{Q}\mathbf{P}. \quad (3.103)$$

The line of reasoning leading to (3.102) cannot be applied to  $\mathbf{H}$  and  $\mathbf{K}$  because there is no position field in  $\mathcal{M}$  associated with material points  $p$ . Instead, we appeal to the aforementioned result in finite-elasticity theory and define superposed rigid-body motions by the requirement that  $W(= \hat{W})$  have the same value at any two  $\mathbf{H}$  related by a superposed rigid-body motion. Let  $\mathbf{H}_1(t)$  and  $\mathbf{H}_2(t)$  be two elastic deformations so related and define  $\mathbf{Z}(t) = \mathbf{H}_2\mathbf{H}_1^{-1}$ . We require that  $\hat{W}(\mathbf{H}_1^T\mathbf{Z}^T\mathbf{Z}\mathbf{H}_1) = \hat{W}(\mathbf{H}_1^T\mathbf{H}_1)$  for  $\mathbf{H}_1 \in Lin$  with  $J_{H_1} > 0$ . To obtain a necessary condition we set  $\mathbf{H}_1 = \mathbf{1}$ , and derive  $\hat{W}(\mathbf{Z}^t\mathbf{Z}) = \hat{W}(\mathbf{1})$ . Our constitutive hypotheses imply that  $\hat{W}(\mathbf{Z}^T\mathbf{Z}) > \hat{W}(\mathbf{1})$  if  $\mathbf{Z}^T\mathbf{Z} \neq \mathbf{1}$ . The two statements are reconciled only if  $\mathbf{Z}^T\mathbf{Z} = \mathbf{1}$  and it follows, since  $J_Z > 0$ , that  $\mathbf{Z} \in Orth^+$ , which is also sufficient. Therefore, in a superposed rigid motion,

$$\mathbf{H} \rightarrow \mathbf{Q}_H\mathbf{H}, \quad (3.104)$$

where  $\mathbf{Q}_H$  is a rotation. Since the argument is local, this rotation may depend on  $\mathbf{x}$  (or  $\mathbf{X}$ ) in addition to  $t$ . It follows immediately from (3.104) that  $\mathbf{C}_H$  and  $\mathbf{S}(\mathbf{C}_H)$  are invariant under superposed rigid motions.

To obtain the transformation rule for the plastic deformation  $\mathbf{K}$ , we assume that superposed rigid motions do not generate dissipation, so that the dissipations associated with any two motions related by a superposed rigid-body motion are identical. Clearly the Eshelby tensor  $\mathbf{E}$  given by (2.205) is invariant under superposed rigid motions. This can

be seen from (2.205) and the invariance of  $\rho_\kappa f$ , which is implied by that of  $W$  and  $J_K$ , the latter following from (3.18), (3.102) and (3.104). Further, from (3.67)<sub>1</sub>, (3.77) and (3.100) we have

$$\mathbf{E}' = \hat{W}(\mathbf{C}_H)\mathbf{1} - \mathbf{C}_H\mathbf{S}(\mathbf{C}_H), \quad (3.105)$$

which is also invariant. Suppose  $\mathbf{K}_1(t)$  and  $\mathbf{K}_2(t)$  are two plastic flows related by a superposed rigid-body motion and let  $\mathbf{Z}(t) = \mathbf{K}_2\mathbf{K}_1^{-1}$ . These generate two local configurations  $\kappa_{i_1}$  and  $\kappa_{i_2}$  from  $\kappa_r$  at  $\mathbf{X}$  via the maps  $\mathbf{K}_1^{-1}$  and  $\mathbf{K}_2^{-1}$ , respectively. We assume the superposed rigid motion to commence at time  $t_0$  so that  $\mathbf{Z}(t_0) = \mathbf{1}$ . If  $D_1 = J_{K_1}^{-1}\mathbf{E}' \cdot \mathbf{K}_1^{-1}\dot{\mathbf{K}}_1$  is the dissipation associated with  $\mathbf{K}_1$  then the dissipation  $D_2$  associated with  $\mathbf{K}_2$  satisfies

$$J_{K_2}D_2 = J_{K_1}D_1 + \mathbf{E}' \cdot \mathbf{K}_1^{-1}\mathbf{Z}^{-1}\dot{\mathbf{Z}}\mathbf{K}_1. \quad (3.106)$$

Invoking the invariance of  $J_K$  and the assumed invariance of the dissipation then yields

$$\mathbf{E}' \cdot \mathbf{K}_1^{-1}\mathbf{Z}^{-1}\dot{\mathbf{Z}}\mathbf{K}_1 = 0, \quad (3.107)$$

for any plastic flow  $\mathbf{K}_1(t)$ . To obtain a necessary condition we set  $\mathbf{K}_1(t) \equiv \mathbf{1}$  at the point  $p$ , which amounts to adopting  $\kappa_{i_1}$  as the reference configuration for the superposed rigid motion, this being permitted by the purely local nature of the argument. This in turn yields  $\mathbf{E}' \cdot \mathbf{Z}^{-1}\dot{\mathbf{Z}} = 0$  and  $\mathbf{Z} \equiv \mathbf{K}_2$ , ensuring that  $\mathbf{Z}(t)$  is a plastic flow. As such it is subject to the dissipation hypothesis (3.87), which is easily seen to be equivalent to the statement:

$$\dot{\mathbf{K}} \neq \mathbf{0} \quad \text{if and only if} \quad \mathbf{E}' \cdot \mathbf{K}^{-1}\dot{\mathbf{K}} > 0. \quad (3.108)$$

It follows that  $\dot{\mathbf{Z}}$  vanishes and hence that  $\mathbf{Z}(t) = \mathbf{Z}(t_0) = \mathbf{1}$ . This is also sufficient for (3.107) and for the invariance of the dissipation. Thus,  $\mathbf{K}_2 = \mathbf{K}_1$  and  $\mathbf{K}$  is invariant under

superposed rigid motions, i.e.

$$\mathbf{K} \rightarrow \mathbf{K}. \quad (3.109)$$

As a corollary, we then have  $\mathbf{Q}_H = \mathbf{Q}(t)$ , implying that  $\mathbf{Q}_H$  is spatially uniform.

In addition to furnishing the transformation rules for the elastic and plastic deformations under superposed rigid motions, the strong dissipation hypothesis and our constitutive hypotheses on the elastic response also imply that plastic evolution ceases in the absence of elastic distortion. For, if  $\mathbf{C}_H = \mathbf{1}$  then  $\hat{W}$  and  $\mathbf{S}$  vanish; therefore  $\mathbf{E}'$  and  $\mathbf{E}$  vanish,  $D = 0$  and (3.87) yields  $\dot{\mathbf{K}} = \mathbf{0}$ .

### 3.6 Material symmetry

The function  $W(\mathbf{H})$  is subject to restrictions imposed by material symmetry. These are of the kind one finds in conventional finite elasticity theory and are crucial to the understanding of elastic/plastic response. Accordingly, a brief review of the concept is appropriate before proceeding. Thus, if two local configurations  $\kappa_{i_1}$  and  $\kappa_{i_2}$  are used to describe the stress  $\mathbf{T}$  at a material point in  $\kappa_t$ , then

$$\mathbf{T} = (W_1)_{\mathbf{H}_1}(\mathbf{H}_1^*)^{-1} \quad \text{and} \quad \mathbf{T} = (W_2)_{\mathbf{H}_2}(\mathbf{H}_2^*)^{-1}, \quad (3.110)$$

where  $W_1(\mathbf{H}_1)$  and  $W_2(\mathbf{H}_2)$  are the associated strain-energy functions. These equations are identical to (3.8). Accordingly, if  $\mathbf{A}$  is a map from  $\kappa_{i_1}$  to  $\kappa_{i_2}$ , then

$$\mathbf{H}_1 = \mathbf{H}_2\mathbf{A}, \quad (3.111)$$

and if  $\mathbf{A}$  is fixed at the material point  $p$ , then consistency between the two expressions for  $\mathbf{T}$  requires that (cf. (3.9))

$$W_1(\mathbf{H}_1) = J_A W_2(\mathbf{H}_2). \quad (3.112)$$

This formula specifies the change in the form of the strain-energy function induced by any local time-independent change of reference at a given material point.

Suppose now that there exists a local change of reference  $\mathbf{G}_1$ , with  $J_{G_1} = 1$ , such that  $W_2(\mathbf{H}) = W_1(\mathbf{H})$  with  $J_H > 0$ ; the two local references then respond identically to a given deformation. Using (3.111), we find that

$$W_1(\mathbf{H}) = W_1(\mathbf{H}\mathbf{G}_1). \quad (3.113)$$

It is well known that the set of all such  $\mathbf{G}_1$  is a group  $\mathcal{G}_1$ , say, the *symmetry group* associated with  $\kappa_{i_1}$ . If the body is materially uniform, then  $W_1(\mathbf{H})$  does not depend explicitly on  $X \in \mathfrak{B}$  (or on  $\mathbf{X} \in \kappa_r$ ). This restriction is satisfied by requiring that  $\mathbf{G}_1$  be independent of  $X \in \mathfrak{B}$  [129, 37].

Combining (3.112) with (3.113), we have

$$J_A W_2(\mathbf{H}) = W_1(\mathbf{H}\mathbf{A}) = W_1(\mathbf{H}\mathbf{A}\mathbf{G}_1) = J_A W_2(\mathbf{H}\mathbf{A}\mathbf{G}_1\mathbf{A}^{-1}). \quad (3.114)$$

In other words,

$$W_2(\mathbf{H}) = W_2(\mathbf{H}\mathbf{G}_2), \quad \text{with} \quad \mathbf{G}_2 = \mathbf{A}\mathbf{G}_1\mathbf{A}^{-1}, \quad (3.115)$$

which is Noll's Rule  $\mathcal{G}_2 = \mathbf{A}\mathcal{G}_1\mathbf{A}^{-1}$  relating the symmetry groups of the two local references.

We have seen in Section 3.1 that our constitutive hypotheses determine the placements of stress-free local equilibrium configurations in  $\mathcal{E}$  modulo orientation and translation.

Thus, if  $\kappa_{i_1}$  is a local relaxed configuration, then any  $\kappa_{i_2}$  is also such a configuration provided that the transformation  $\mathbf{A}$  from  $\kappa_{i_1}$  to  $\kappa_{i_2}$  is a rotation. Further,  $\mathcal{G}_1$  is a subgroup of the orthogonal group if and only if the same is true of  $\mathcal{G}_2$ . Any  $\mathbf{G}_2 \in \mathcal{G}_2$  is obtained simply by rotating some  $\mathbf{G}_1 \in \mathcal{G}_1$  by  $\mathbf{A}$  to obtain  $\mathbf{G}_2 = \mathbf{A}\mathbf{G}_1\mathbf{A}^T$ . For example, if  $\mathbf{e}_i$  ( $i \in \{1, 2, 3\}$ ) are the orthonormal axes of a cubic lattice in  $\kappa_{i_1}$ , then the  $180^\circ$  rotation  $\mathbf{G}_1 = 2\mathbf{e}_3 \otimes \mathbf{e}_3 - \mathbf{1}$  about  $\mathbf{e}_3$  maps the lattice to itself and thus belongs to  $\mathcal{G}_1$ . The corresponding element of  $\mathcal{G}_2$  is given by  $\mathbf{G}_2 = 2\mathbf{e}'_3 \otimes \mathbf{e}'_3 - \mathbf{1}$ , where  $\mathbf{e}'_i = \mathbf{A}\mathbf{e}_i$ .

This result is of the greatest importance for the practical implementation of the theory. It implies that the symmetry group  $\mathcal{G}_1$  for the local stress-free  $\kappa_{i_1}$  may be fixed once and for all, provided that this group is a sub-group of the orthogonal group. Then, given the response function  $W_1(\mathbf{H})$ , we generate the response function relative to any relaxed local configuration  $\kappa_{i_2}$  by setting  $W_2(\mathbf{H}) = W_1(\mathbf{H}\mathbf{A})$ , where  $\mathbf{A}$  is a suitable rotation. By construction, all such configurations are equivalent insofar as the computation of the stress is concerned. The same issue is discussed from a different viewpoint in [168].

For example, if the material in configuration  $\kappa_i$  exhibits cubic symmetry, and if the elastic strain is sufficiently small to justify a quadratic approximation to the energy, then the strain-energy function is of the form [60]

$$\hat{W} = \frac{1}{2}C_1(\epsilon_{11} + \epsilon_{22} + \epsilon_{33})^2 + C_2(\epsilon_{11}\epsilon_{22} + \epsilon_{11}\epsilon_{33} + \epsilon_{22}\epsilon_{33}) + C_3(\epsilon_{12}^2 + \epsilon_{13}^2 + \epsilon_{23}^2), \quad (3.116)$$

where  $C_i; i = \{1, 2, 3\}$  are material constants,  $\epsilon_{ij} = \boldsymbol{\epsilon} \cdot \text{Sym}(\mathbf{e}_i \otimes \mathbf{e}_j)$ ,  $\{\mathbf{e}_i\} \in \mathcal{V}$  is a basis of orthonormalized vectors aligned with the cube axes, and

$$\boldsymbol{\epsilon} = \frac{1}{2}(\mathbf{C}_H - \mathbf{1}) \quad (3.117)$$

is the (infinitesimal) elastic strain. The linear and quadratic invariants of  $\boldsymbol{\epsilon}$  are common to

each of the five subclasses of cubic symmetry [60]. Accordingly, (3.116) applies to all kinds of cubic symmetry. From (3.101) we then obtain

$$\begin{aligned} \mathbf{S} = & C_1(\text{tr } \boldsymbol{\epsilon})\mathbf{1} + C_2[(\epsilon_{22} + \epsilon_{33})\mathbf{e}_1 \otimes \mathbf{e}_1 + (\epsilon_{11} + \epsilon_{33})\mathbf{e}_2 \otimes \mathbf{e}_2 + (\epsilon_{11} + \epsilon_{22})\mathbf{e}_3 \otimes \mathbf{e}_3] \\ & + C_3[\epsilon_{12}(\mathbf{e}_1 \otimes \mathbf{e}_2 + \mathbf{e}_2 \otimes \mathbf{e}_1) + \epsilon_{13}(\mathbf{e}_1 \otimes \mathbf{e}_3 + \mathbf{e}_3 \otimes \mathbf{e}_1) + \epsilon_{23}(\mathbf{e}_2 \otimes \mathbf{e}_3 + \mathbf{e}_3 \otimes \mathbf{e}_2)]. \end{aligned} \quad (3.118)$$

Our requirement that  $\hat{W}$  be a convex function of  $\mathbf{C}_H$  is satisfied if and only if it is a convex function of  $\boldsymbol{\epsilon}$ . In the quadratic case this in turn is satisfied if and only if the energy is a positive-definite function of  $\boldsymbol{\epsilon}$ . To construct necessary conditions for this, we set all  $\epsilon_{ij} = 0$  except  $\epsilon_{12}(= \epsilon_{21})$ . The resulting inequality can then be satisfied only if  $C_3 > 0$ , which in turn ensures that the final quadratic form in (3.116) is positive definite. Next, we set all off-diagonal components  $\epsilon_{ij}$  to zero, along with  $\epsilon_{33}$ . We then require

$$\frac{1}{2}C_1(\epsilon_{11} + \epsilon_{22})^2 + C_2\epsilon_{11}\epsilon_{22} > 0 \quad (3.119)$$

for all  $\epsilon_{11}, \epsilon_{22}$ . For this it is necessary and sufficient that  $C_1 > 0$  and  $C_2 \in (-2C_1, 0)$ . Necessary conditions for positive-definiteness are thus given by

$$C_1 > 0, \quad C_3 > 0, \quad -2C_1 < C_2 < 0. \quad (3.120)$$

To derive sufficient conditions we write (3.116) in the form

$$\hat{W} = P(\epsilon_{11}, \epsilon_{22}) + P(\epsilon_{11}, \epsilon_{33}) + P(\epsilon_{22}, \epsilon_{33}) + C_3(\epsilon_{12}^2 + \epsilon_{13}^2 + \epsilon_{23}^2), \quad (3.121)$$

where

$$P(A, B) = \frac{1}{4}C_1(A^2 + B^2) + (C_1 + C_2)AB. \quad (3.122)$$

Sufficient conditions for positive-definiteness are  $C_3 > 0$  and  $P(A, B) > 0$ , which holds if and only if  $C_1 > 0$  and  $C_1^2 > 4(C_1 + C_2)^2$ . The latter are equivalent to  $C_1/2 > |C_1 + C_2|$ .

Taken together we have

$$C_1 > 0, \quad C_3 > 0, \quad -\frac{3}{2}C_1 < C_2 < -\frac{1}{2}C_1. \quad (3.123)$$

From the foregoing discussion it is clear that, in the presence of convexity, the response functions relative to any other stress-free local configuration are obtained from those given simply by substituting  $\mathbf{e}'_i = \mathbf{A}\mathbf{e}_i$  in place of  $\mathbf{e}_i$ , where  $\mathbf{A}$  is a suitable rotation. Accordingly, since these configurations are, by construction, equivalent insofar as the computation of the stress in  $\kappa_t$  is concerned, we may fix the basis  $\{\mathbf{e}_i\}$ , and hence the symmetry group  $\mathcal{G}_{\kappa_i}$ , once and for all. For example, we may identify  $\mathbf{e}_i$  with their values in some known configuration of the body, which may then serve as a reference configuration  $\kappa_r$ . This is not to say that we identify  $\kappa_i$  with  $\kappa_r$ ; rather, we simply require that  $\mathcal{G}_{\kappa_i}$  be insensitive to plastic flow, as suggested by experiments on crystal slip [162, 93]. Similar ideas are imposed *a priori* as part of the definition of plastic deformation in [168, 115, 125].

In the isotropic case the quadratic approximation to the strain-energy function and the associated expression for the stress are, of course, well known. Thus,

$$\hat{W} = \frac{1}{2}\lambda(\text{tr } \boldsymbol{\epsilon})^2 + \mu \boldsymbol{\epsilon} \cdot \boldsymbol{\epsilon} \quad \text{and} \quad \mathbf{S} = \lambda(\text{tr } \boldsymbol{\epsilon})\mathbf{1} + 2\mu\boldsymbol{\epsilon}, \quad (3.124)$$

where  $\lambda$  and  $\mu$  are the Lamé moduli. Necessary and sufficient conditions for convexity are that  $\mu > 0$  and  $\lambda + \frac{2}{3}\mu > 0$ .



## 3.7 Flow and yield

In this section we obtain the general forms of the flow rule and the yield condition, after imposing restrictions of invariance under the change of reference configuration, invariance under a rigid body motion, and considerations of material symmetry.

### 3.7.1 Flow rule

To complete the model we require a flow rule for the evolution of plastic deformation  $\mathbf{K}$ . In view of the structure of the dissipation inequality (3.75), it is natural to consider rules of the form

$$\mathcal{F}(\mathbf{K}^{-1}, \dot{\mathbf{K}}^{-1}, \mathbf{H}, \dot{\mathbf{H}}, \mathbf{E}, \dot{\mathbf{E}}, \nabla \mathbf{K}^{-1}, \theta, \dot{\theta}, \mathbf{g}) = \mathbf{0}, \quad (3.125)$$

where  $\mathcal{F} : \kappa_i \rightarrow \kappa_i$  is a tensor-valued function. It is assumed in line with our assumption of material uniformity, that this function does not depend explicitly on  $p = \kappa_i(X)$ .

Following [45], we impose the requirement that this equation be invariant under compatible changes of the reference configuration  $\kappa_r$ . The reason for this is that the choice of reference is in principle a matter of convenience and hence irrelevant to the physical processes under study. Precisely the same viewpoint was adopted in the derivation of (3.9) by invoking the insensitivity of the Cauchy stress to the choice of reference. We have obtained in Section 3.3 the necessary and sufficient conditions for the representation of constitutive functions to be invariant under compatible changes in the reference configuration. Before using the result from Section 3.3, recall from (3.76), that,  $\mathbf{E} = J_K^{-1} \mathbf{K}^{-T} \mathbf{E}' \mathbf{K}^T$ , where  $\mathbf{E}' = W \mathbf{1} - \mathbf{H}^T W_{\mathbf{H}}$  and  $W = \tilde{W}(\mathbf{H})$ . We can in addition obtain

$$J_K \mathbf{K}^T \dot{\mathbf{E}} \mathbf{K}^{-T} = \dot{\mathbf{E}}' + \mathbf{E}' (\mathbf{K}^{-1} \dot{\mathbf{K}})^T - (\mathbf{K}^{-1} \dot{\mathbf{K}})^T \mathbf{E}' - \mathbf{E}' \text{tr}(\mathbf{K}^{-1} \dot{\mathbf{K}}). \quad (3.126)$$

Noting (3.77), the function  $\mathcal{F}$  can therefore be equivalently represented as

$$\mathcal{F}(\mathbf{K}^{-1}, \dot{\mathbf{K}}^{-1}, \mathbf{H}, \dot{\mathbf{H}}, \mathbf{E}, \dot{\mathbf{E}}, \nabla \mathbf{K}^{-1}, \theta, \dot{\theta}, \mathbf{g}) = \tilde{\mathcal{F}}(\mathbf{K}^{-1}, \dot{\mathbf{K}}^{-1}, \mathbf{H}, \dot{\mathbf{H}}, \nabla \mathbf{K}^{-1}, \theta, \dot{\theta}, \mathbf{g}). \quad (3.127)$$

The set of variables are now similar to that considered in Section 3.3 and we can use the result obtain therein to conclude the following representation for flow rule

$$\hat{\mathcal{F}}(\mathbf{H}, \dot{\mathbf{H}}, \mathbf{K}^{-1} \mathbf{K}, \boldsymbol{\alpha}, \theta, \dot{\theta}, \mathbf{g} \mathbf{K}) = \mathbf{0}. \quad (3.128)$$

Further, if we impose the invariance of the function  $\hat{\mathcal{F}}$  under superposed rigid-body motions then it is unaffected by the substitution of  $\mathbf{Q}(t)\mathbf{H}$  in place of  $\mathbf{H}$ . Equating  $\mathbf{Q}^T$  identically to the rotation in the polar factorization of  $\mathbf{H}$ , we then have the flow rule as

$$\check{\mathcal{F}}(\mathbf{C}_H, \dot{\mathbf{C}}_H, \mathbf{K}^{-1} \mathbf{K}, \boldsymbol{\alpha}, \theta, \dot{\theta}, \mathbf{g} \mathbf{K}) = \mathbf{0}. \quad (3.129)$$

This form of the flow rule provides us with the necessary and sufficient condition for it to be invariant under compatible changes in the reference configuration and also under rigid body motions. A special case of (3.129) has the form

$$\dot{\mathbf{K}}^{-1} \mathbf{K} = \mathcal{H}(\mathbf{C}_H, \dot{\mathbf{C}}_H, \boldsymbol{\alpha}, \theta, \dot{\theta}, \mathbf{g} \mathbf{K}). \quad (3.130)$$

**Plastic spin** We observe from (3.105) that  $\mathbf{M}(\mathbf{C}_H) \in \text{Sym}$ , where

$$\mathbf{M}(\mathbf{C}_H) = \mathbf{E}' \mathbf{C}_H. \quad (3.131)$$

To embed this fact in the model, assume the response to be isothermal and write the dissipation (cf. (3.78), without the heat term) in the form

$$J_K D = \mathbf{M} \cdot \mathbf{K}^{-1} \dot{\mathbf{K}} \mathbf{C}_H^{-1}. \quad (3.132)$$

Hypothesis (3.87) is then equivalent to the statement

$$\dot{\mathbf{K}} \neq \mathbf{0} \quad \text{if and only if} \quad \mathbf{M} \cdot \mathbf{K}^{-1} \dot{\mathbf{K}} \mathbf{C}_H^{-1} > 0. \quad (3.133)$$

It follows immediately that  $\dot{\mathbf{K}}$  vanishes if  $\mathbf{K}^{-1} \dot{\mathbf{K}} \mathbf{C}_H^{-1} \in Skw$ . In other words, the latter does not correspond to a *bona fide* evolution of plasticity. Conversely, if  $\dot{\mathbf{K}} \neq \mathbf{0}$  then  $\mathbf{K}^{-1} \dot{\mathbf{K}} \mathbf{C}_H^{-1}$  is not skew. This of course should not be construed to mean that that latter is symmetric. However, it does beg the question of how the skew part of  $\mathbf{K}^{-1} \dot{\mathbf{K}} \mathbf{C}_H^{-1}$  should be interpreted. This is the issue of *plastic spin*, which is of significant ongoing concern in the plasticity literature (e.g. [168, 109, 166]). To address it, we exploit the latitude afforded by the constitutive character of  $\mathbf{K}$  and adopt the *constitutive* assumption

$$\mathbf{K}^{-1} \dot{\mathbf{K}} \mathbf{C}_H^{-1} \in Sym. \quad (3.134)$$

In effect, we resolve the issue simply by requiring that indeterminate variables vanish.

The flow rule (3.130) simplifies accordingly. Using  $\dot{\mathbf{K}}^{-1} \mathbf{K} = -\mathbf{K}^{-1} \dot{\mathbf{K}}$ , we have

$$\mathbf{K}^{-1} \dot{\mathbf{K}} \mathbf{C}_H^{-1} = \mathcal{S}(\mathbf{C}_H, \dot{\mathbf{C}}_H, \boldsymbol{\alpha}), \quad (3.135)$$

where

$$\mathcal{S}(\mathbf{C}_H, \dot{\mathbf{C}}_H, \boldsymbol{\alpha}) = \mathcal{H}(\mathbf{C}_H, \dot{\mathbf{C}}_H, \boldsymbol{\alpha}) \mathbf{C}_H^{-1} \in Sym. \quad (3.136)$$

The plastic deformation then satisfies

$$\dot{\mathbf{K}} = \mathbf{K} \mathcal{S}(\mathbf{C}_H, \dot{\mathbf{C}}_H, \boldsymbol{\alpha}) \mathbf{C}_H. \quad (3.137)$$

The specialization to rate-independent response is of particular interest in applications. In this case we require the flow rule to be insensitive to the time scale, so that  $\mathcal{S}$

is homogenous of degree one in its second argument, i.e.

$$\mathcal{S}(\mathbf{C}_H, \lambda \dot{\mathbf{C}}_H, \boldsymbol{\alpha}) = \lambda \mathcal{S}(\mathbf{C}_H, \dot{\mathbf{C}}_H, \boldsymbol{\alpha}) \quad \text{for all } \lambda \in \mathbb{R}. \quad (3.138)$$

Differentiating with respect to  $\lambda$  and evaluating the result at  $\lambda = 0$  furnishes the necessary and sufficient condition

$$\mathcal{S}(\mathbf{C}_H, \dot{\mathbf{C}}_H, \boldsymbol{\alpha}) = \mathcal{M}(\mathbf{C}_H, \boldsymbol{\alpha})[\dot{\mathbf{C}}_H], \quad (3.139)$$

where  $\mathcal{M}$  is a fourth-order tensor.

**Material symmetry** It is obvious from its structure that the function  $\mathcal{S}$  (or  $\mathcal{H}$ ) depends on the local configuration  $\kappa_i$ . We are concerned with material symmetry and thus with the question of how the flow rule transforms under variations of these configurations. The role of material symmetry in this context is discussed in the comprehensive review by Cleja-Țigoiu and Soos [168] and independently by Epstein [45].<sup>16</sup> Thus, consider a map from  $\kappa_{i_1}$  to  $\kappa_{i_2}$ , as in Section 3.6. Assume  $\mathbf{x} = \boldsymbol{\chi}(\mathbf{X}, t)$  to be given. Using (3.18) and (3.111) for fixed  $\mathbf{F}$ , we have

$$\mathbf{K}_1 = \mathbf{K}_2 \mathbf{A}. \quad (3.140)$$

Writing (3.137) for both local configurations, we are then led, using obvious notation, to the rule

$$\mathcal{S}_2(\mathbf{C}_{H_2}, \dot{\mathbf{C}}_{H_2}, \boldsymbol{\alpha}_2) = \mathbf{A} \mathcal{S}_1(\mathbf{C}_{H_1}, \dot{\mathbf{C}}_{H_1}, \boldsymbol{\alpha}_1) \mathbf{A}^T, \quad (3.141)$$

where, for  $\mathbf{A}$  fixed at  $p$ , as in Section 3.6,

$$\mathbf{C}_{H_1} = \mathbf{A}^T \mathbf{C}_{H_2} \mathbf{A} \quad \text{and} \quad \dot{\mathbf{C}}_{H_1} = \mathbf{A}^T \dot{\mathbf{C}}_{H_2} \mathbf{A}. \quad (3.142)$$

---

<sup>16</sup>The role of material symmetry in a theory of polymer science based on local intermediate configurations is discussed in [177, 148].

we use (3.23)<sub>1</sub> to relate  $\alpha_1$  to  $\alpha_2$ . Thus,

$$\alpha_1 = J_{K_1} \mathbf{K}_1^{-1} \text{Curl} \mathbf{K}_1^{-1} = J_A J_{K_2} \mathbf{A}^{-1} \mathbf{K}_2^{-1} \text{Curl}(\mathbf{A}^{-1} \mathbf{K}_2^{-1}). \quad (3.143)$$

If the change of local reference is uniform, in the sense that  $\mathbf{A}$  is independent of  $p$  (hence, of  $\mathbf{X}$ ), we have [30]

$$\text{Curl}(\mathbf{A}^{-1} \mathbf{K}_2^{-1}) = (\text{Curl} \mathbf{K}_2^{-1}) \mathbf{A}^{-T}, \quad (3.144)$$

yielding

$$\alpha_1 = J_A \mathbf{A}^{-1} \alpha_2 \mathbf{A}^{-T}. \quad (3.145)$$

Thus, if the function  $\mathcal{S}_1$  is known, then  $\mathcal{S}_2$  is generated by the formula

$$\mathcal{S}_2(\mathbf{C}_H, \dot{\mathbf{C}}_H, \alpha) = \mathbf{A} \mathcal{S}_1(\mathbf{A}^T \mathbf{C}_H \mathbf{A}, \mathbf{A}^T \dot{\mathbf{C}}_H \mathbf{A}, J_A \mathbf{A}^{-1} \alpha \mathbf{A}^{-T}) \mathbf{A}^T. \quad (3.146)$$

Since the local configurations  $\kappa_{i_1}$  and  $\kappa_{i_2}$  are stress-free by definition, our constitutive hypotheses give  $\mathbf{A} \in \text{Orth}^+$ , affording the simplification

$$\mathcal{S}_2(\mathbf{C}_H, \dot{\mathbf{C}}_H, \alpha) = \mathbf{A} \mathcal{S}_1(\mathbf{A}^T \mathbf{C}_H \mathbf{A}, \mathbf{A}^T \dot{\mathbf{C}}_H \mathbf{A}, \mathbf{A}^T \alpha \mathbf{A}) \mathbf{A}^T. \quad (3.147)$$

Suppose now that the transformation is such that both local references respond identically. Let  $\mathbf{G}_1$  be such a transformation. Then the functions  $\mathcal{S}_1$  and  $\mathcal{S}_2$  coincide, and (3.147) furnishes

$$\mathbf{G}_1^T \mathcal{S}_1(\mathbf{C}_H, \dot{\mathbf{C}}_H, \alpha) \mathbf{G}_1 = \mathcal{S}_1(\mathbf{G}_1^T \mathbf{C}_H \mathbf{G}_1, \mathbf{G}_1^T \dot{\mathbf{C}}_H \mathbf{G}_1, \mathbf{G}_1^T \alpha \mathbf{G}_1). \quad (3.148)$$

Here we identify  $\mathbf{G}_1$  with any element of  $\mathcal{G}_1$ , the symmetry group associated with  $\kappa_{i_1}$ . The restriction to uniform  $\mathbf{A}$  (hence uniform  $\mathbf{G}_1$ ) is due to our prescription for enforcing the condition of material uniformity in Section 3.6.

It is easily demonstrated that the dissipation  $J_K D$  regarded as a function of the variables  $\mathbf{C}_H, \dot{\mathbf{C}}_H$ , and  $\boldsymbol{\alpha}$ , is invariant under symmetry transformations. Further, a straightforward but involved calculation based on (3.146) and (3.148) furnishes the analog of Noll's rule for plastic flow, which we do not record here.

In practice, given  $\mathcal{G}_1$ , (3.148) is solved by regarding  $\mathcal{S}$  as a function of three symmetric tensors and one vector [178]. This reduction is achieved by writing  $\mathcal{S}$  as a function of  $Sym(\boldsymbol{\alpha})$  and  $Skw(\boldsymbol{\alpha})$ . If  $\mathbf{a}$  is the axial vector of  $Skw(\boldsymbol{\alpha})$ , then  $\mathbf{G}^T Skw(\boldsymbol{\alpha}) \mathbf{G}$  may be replaced by  $\mathbf{G}^T \mathbf{a}$  in the statement of material symmetry, for any  $\mathbf{G} \in \mathcal{G}_1 \subset Orth^+$ . To see this we observe that for any vector  $\mathbf{u}$ ,

$$\mathbf{G}^T \mathbf{a} \times \mathbf{G}^T \mathbf{u} = \mathbf{G}^T (\mathbf{a} \times \mathbf{u}) = \mathbf{G}^T Skw(\boldsymbol{\alpha}) \mathbf{u} = [\mathbf{G}^T Skw(\boldsymbol{\alpha}) \mathbf{G}] (\mathbf{G}^T \mathbf{u}), \quad (3.149)$$

so that  $\mathbf{G}^T \mathbf{a}$  is the axial vector of  $\mathbf{G}^T Skw(\boldsymbol{\alpha}) \mathbf{G}$ . With this simplification, the problem of solving (3.148) for the canonical form of the response function is tractable [178]. It is eased considerably in the rate independent case in which the functional dependence on  $\dot{\mathbf{C}}_H$  is linear.

*Remark 3.7.1.* In the case of isotropy,  $\mathbf{C}_H$  commutes with  $\mathbf{S}(\mathbf{C}_H)$  so that  $\mathbf{E}' \in Sym$ . It follows from (3.108) and the argument leading from (3.133) to (3.134) that if  $\dot{\mathbf{K}} \neq \mathbf{0}$ , then  $\mathbf{K}^{-1} \dot{\mathbf{K}} \in Sym$ , and thus from (3.135) that  $\mathcal{S}$  also commutes with  $\mathbf{C}_H$ . This means that  $\mathcal{H} \in Sym$ , where  $\mathcal{H}$  is now a hemitropic function of its arguments. In the case of isotropy an independent argument, relying on the connectedness of the symmetry group, may be used to eliminate the plastic spin  $Skw(\mathbf{K}^{-1} \dot{\mathbf{K}})$ . This is discussed in [48]. A variant of the idea is developed independently in [69]. However, the present model, in which dislocation density figures in the list of variables, is not appropriate in the case of isotropy. This is

due to the degree of freedom  $\mathbf{H} \rightarrow \mathbf{H}\mathbf{G}$  afforded by material symmetry. If  $\mathbf{G}$  belongs to a continuous group, as in the case of isotropy or transverse isotropy, then the dislocation density is highly non-unique and is therefore not a state variable. The issue is discussed in ([129], Theorem 8) and investigated in [37]. There is no such difficulty in the case of a discrete group, however. In the isotropic case, Riemannian curvature derived from the plastic strain furnishes a unique measure of defectiveness of the material. The associated theory entails significant complications vis à vis that considered here [46]. We will take up this aspect of the theory again in Remark 3.8.3 in the next section, where we also discuss, the restrictions thus imposed on our model.

**Motion of a single dislocation** Following Kosevich [90] and Mura [120], we write down the flow rule for a single dislocation line  $L \subset \kappa_r$  moving with velocity  $\mathbf{V} \in \mathcal{V}$  as

$$\dot{\mathbf{K}}^{-1} = \mathbf{b} \otimes (\boldsymbol{\delta}(L) \times \mathbf{V}), \quad (3.150)$$

where  $\mathbf{b} \in T_{\mathcal{M}}$  is the constant Burgers vector and  $\boldsymbol{\delta}(L)$  is a generalized function defined in (3.31). Assuming the thermodynamic response to be isothermal, the net dissipation as a result of the motion of a single dislocation can be calculated from integrating (3.85) over  $\kappa_r$ . Use (3.76), (3.77), and  $\dot{\mathbf{K}}^{-1}\mathbf{K} = -\mathbf{K}^{-1}\dot{\mathbf{K}}$  in (3.85) to obtain

$$\int_{\kappa_r} J_K^{-1} \mathbf{E}' \cdot \dot{\mathbf{K}}^{-1} \mathbf{K} dV < 0. \quad (3.151)$$

Note from (3.150) that

$$\begin{aligned} \dot{\mathbf{K}}^{-1} \mathbf{K} &= \mathbf{b} \otimes \mathbf{K}^T (\boldsymbol{\delta}(L) \times \mathbf{V}) \\ &= J_K \mathbf{b} \otimes (\mathbf{K}^{-1} \boldsymbol{\delta}(L) \times \mathbf{K}^{-1} \mathbf{V}), \end{aligned} \quad (3.152)$$

where the second equality has been obtained using the definition of cofactor from (2.24) and (2.25). Substitute (3.152) into (3.151) and use (3.31) to get

$$\int_L \mathbf{E}' \cdot \mathbf{b} \otimes (\mathbf{K}^{-1}\mathbf{t} \times \mathbf{K}^{-1}\mathbf{V}) dL < 0, \quad (3.153)$$

where  $\mathbf{t} \in \mathcal{V}$  denotes the tangent to the dislocation line  $L$ . The vectors  $\{\hat{\mathbf{t}}, \hat{\mathbf{V}}\} \in T_{\mathcal{M}}$  defined by

$$\hat{\mathbf{t}} = \mathbf{K}^{-1}\mathbf{t}, \quad \text{and} \quad \hat{\mathbf{V}} = \mathbf{K}^{-1}\mathbf{V} \quad (3.154)$$

denote the tangent and velocity associated with the dislocation line, respectively, in the intermediate configuration. Using these definitions, (3.153) can be rewritten as

$$\int_L \mathbf{E}' \cdot \mathbf{b} \otimes (\hat{\mathbf{t}} \times \hat{\mathbf{V}}) dL < 0, \quad (3.155)$$

which after some further manipulation yields

$$\int_L (\mathbf{E}'^T \mathbf{b} \times \hat{\mathbf{t}}) \cdot \hat{\mathbf{V}} dL < 0. \quad (3.156)$$

The dissipative force which *drives* the dislocation with velocity  $\hat{\mathbf{V}}$  is therefore

$$\mathbf{f} = \mathbf{E}'^T \mathbf{b} \times \hat{\mathbf{t}}. \quad (3.157)$$

For small elastic strain, the Eshelby tensor  $\mathbf{E}'$  reduces to Cauchy stress, thereby reducing  $\mathbf{f}$  to the expression for Peach-Koehler force [164]. Equation (3.157) provides us with a generalization of Peach-Koehler force to the case of finite elastic strain.

For isochoric plastic flow,  $J_K = 1$  and therefore  $\text{tr} \mathbf{K}^{-1}\dot{\mathbf{K}} = 0$  or  $\text{tr} \mathbf{K}^{-1}\mathbf{K} = 0$ . Equation (3.152) then implies that

$$\delta(L)\mathbf{b} \cdot (\hat{\mathbf{t}} \times \hat{\mathbf{V}}) = 0, \quad (3.158)$$



where we have used definitions (3.154) and the identity  $\boldsymbol{\delta}(L) = \delta(L)\mathbf{t}$ . According to (3.158), the motion of dislocation for an isochoric plastic flow is restricted to the slip plane, i.e.  $\hat{\mathbf{V}}$  lies in the plane spanned by vectors  $\mathbf{b}$  (slip direction) and  $\hat{\mathbf{t}}$  (dislocation line direction).

Finally, we can use the volume average, as introduced in Subsection 3.2.3, to obtain a macroscopic plastic distortion rate. As before, let there be  $a$  types of dislocations in a RVE of volume  $V$ . Define the average plastic distortion rate as

$$\overline{\dot{\mathbf{K}}^{-1}\mathbf{K}} = \frac{1}{V} \int_V \sum_{\xi=1}^a \mathbf{K}^{-1(\xi)} \dot{\mathbf{K}}^{(\xi)} dV, \quad (3.159)$$

which for isochoric plastic flow, takes the form

$$\overline{\dot{\mathbf{K}}^{-1}\mathbf{K}} = \sum_{\xi=1}^a \dot{\gamma}^{(\xi)} \mathbf{s}^{(\xi)} \otimes \hat{\mathbf{N}}^{(\xi)}, \quad (3.160)$$

where

$$\dot{\gamma}^{(\xi)} = \frac{L^{(\xi)}}{V} |\mathbf{b}^{(\xi)}| \cdot |\hat{\mathbf{t}}^{(\xi)} \times \hat{\mathbf{V}}^{(\xi)}|, \quad \text{and } \mathbf{s}^{(\xi)} = \frac{\mathbf{b}^{(\xi)}}{|\mathbf{b}^{(\xi)}|}. \quad (3.161)$$

Here  $L^{(\xi)}$  denotes the length of the dislocation type  $\xi$  inside the RVE and  $\hat{\mathbf{N}}^{(\xi)} \in T_{\mathcal{M}}$  is the fixed unit normal to the slip plane of each dislocation type. Relations (3.160) and (3.161) follow from (3.159) on using equation (3.152) and noting that for isochoric plastic flow,  $\hat{\mathbf{V}}$  lies in the plane of slip. The flow rule in the form (3.160) is used extensively in the theory of crystal plasticity. One should however be cautious on the generality of such a rule. For example, a simple volume averaging like (3.159) might be insufficient to capture the nonlinear effects due to large plastic distortions, thus warranting a more complicated averaging technique.

### 3.7.2 Yield criteria

Conventionally, flow is considered to be possible only if the material is in a state of yield. This is enforced by requiring the pertinent variables to belong to a certain manifold, assumed here to be expressible in the form

$$g(\mathbf{K}^{-1}, \mathbf{H}, \mathbf{E}, \nabla \mathbf{K}^{-1}, \theta) = 0, \quad (3.162)$$

which is preserved by compatible changes of reference configuration and by superposed rigid-body motions. From the foregoing it is immediate that such invariance yields the reduced form

$$g = \hat{g}(\mathbf{C}_H, \boldsymbol{\alpha}, \theta), \quad (3.163)$$

which is subject to the restriction

$$\hat{g}(\mathbf{C}_H, \boldsymbol{\alpha}, \theta) = \hat{g}(\mathbf{G}^T \mathbf{C}_H \mathbf{G}, \mathbf{G}^T \boldsymbol{\alpha} \mathbf{G}, \theta) \quad (3.164)$$

due to material symmetry, this being meaningful only if the symmetry group is discrete (i.e. for crystal symmetry). Further, we assume the response to be elastic, in the sense that  $\dot{\mathbf{K}} = \mathbf{0}$  for all  $\mathbf{C}_H$ ,  $\boldsymbol{\alpha}$  and  $\theta$  such that  $\hat{g} < 0$ . This elastic range is assumed to contain  $\mathbf{C}_H = \mathbf{1}$  for consistency with our earlier finding that plastic flow vanishes in the absence of elastic distortion.

Often further constitutive hypotheses are introduced which lead to a relationship between the yield function and flow rule. We consider these and their implications in the next chapter.

### 3.8 Remarks

*Remark 3.8.1.* (Work hardening) In 1934, Taylor [162] introduced the idea of dependence of the yield strength of a crystal on its dislocation content. He suggested that during plastic flow, many dislocations remain stuck inside the crystal (due to mutual interactions, pile-ups, mosaic boundaries, etc.) and thereby increase its yield strength. This phenomenon of strengthening is referred to as work hardening<sup>17</sup> (also called strain hardening). It has been observed that work hardening depends on the microstructure developed during plastic flow and also on the various structures (patterns), into which dislocations arrange themselves. Owing to much complexity of the phenomenon, most of the progress has been experimental in nature, with very few theoretical considerations. Not surprisingly, the problem of work hardening is seen to be one of the most challenging problems in plasticity theory [123].

In our formulation, we allow for hardening through the dependence of flow rules and yield criteria on the dislocation density tensor (cf. (3.137) and (3.163)). Recalling our discussion on GND and SSD from Subsection 3.2.3, we note that depending on the scale at which plastic distortion is considered, the dislocation density tensor  $\alpha$  associated with GND might lack some information about the microstructure. Moreover, there might be other parameters useful in characterizing hardening, such as those considered in conventional plasticity theories [109]. Additional variables can therefore be added in the constitutive functions for flow and yield. The nature of these internal variables, however, remains ambiguous. We, therefore, will restrict our attention to the forms considered in (3.137) and

---

<sup>17</sup>Excellent introductory account of work hardening can be found in the book by Cottrell [38]. The present state of knowledge in this discipline can be gathered from a special issue on work hardening, which appeared recently in the famous *Dislocations in Solids* series edited by Nabarro [123].

(3.163).

*Remark 3.8.2.* (Size effects and gradient theories of plasticity) The last decade has seen an increasing number of papers in plasticity modeling with an aim to predict size effects,<sup>18</sup> with GND (i.e.  $\alpha$ ) playing the central role. GND has a dimension of reciprocal length, and therefore has been used to induce an internal length scale in the theory. The inclusion of GND has been either through a full strain gradient theory, with free energy depending on GND [68] and the appearance of couples [52], or through a presence in flow rules and yield criteria [2], a view taken in the current work. The latter approach avoids the consideration of additional boundary conditions and complicated free energy functions. However, as pointed out by Mughrabi [119] in his sharp critique of these existing gradient theories, much caution and a closer analysis is needed before a model is put up for predictions. He asks for a better understanding of the microstructure in formulating phenomenological laws, and in particular, for a clear (measurable) meaning of the internal length scale, which “remains vague”.

To discuss this last point, recall Subsections 3.2.2 and 3.2.3. First, consider a theory where plastic distortions are given at the scale of individual dislocations. Then  $\alpha$  characterizes the total dislocation content in the body. Taking a clue from the representation (3.36) for single dislocations, we note that the material length scale introduced by  $\alpha$  is through the Burgers vector  $\mathbf{b}$  and the generalized function  $\delta(L)$ . It is clear from (3.27) and (3.31) that the magnitude of vector  $\delta(L)$  (which is  $\delta(L)$ ) represents the line length of the dislocation per unit volume (use  $\phi = 1$  in (3.27) to reach this conclusion). The

---

<sup>18</sup>Almost all of these papers rest on the experimental investigations by Fleck et al. [52], Stölken and Evans [160], and Nix and Gao [127], the conclusion being *the smaller, the stronger*.

dislocation density, therefore, introduces a *local* length scale of the order  $b\hat{L}$ , where  $b$  and  $\hat{L}$  denote magnitude of the Burgers vector and the dislocation line length per unit volume, respectively. We emphasize the local nature of this scale, which of course varies from one dislocation to another, and therefore from one material point to another. On the other hand, if we consider the plastic distortion as an averaged quantity (over some RVE), we introduce additional length scales (associated with averaging) in the model. An appropriate dependence on SSD will be then required (see also previous remark) to capture the relevant length scales in the theory.

*Remark 3.8.3.* (Continuous and discrete symmetry groups) Following Noll [129], we say the body is *materially uniform*, if material at any two points of the body is same. We will identify the manifold  $\mathcal{M}$ , which is the collection of intermediate configurations, as the body. Consider two points,  $\{p_1, p_2\} \in \mathcal{M}$ . Then,  $\Phi : T_{\mathcal{M}(p_1)} \rightarrow T_{\mathcal{M}(p_2)}$  is called a material isomorphism if

$$\mathfrak{g}_{p_1}(\mathbf{H}(p_1)) = \mathfrak{g}_{p_2}(\mathbf{H}(p_1)\Phi), \quad (3.165)$$

where  $\mathfrak{g}$  is any elastic response functional (for example, Cauchy stress). According to condition (3.165), the elastic response of the material at two points  $p_1$  and  $p_2$  in the body is identical for a given elastic distortion. The isomorphism  $\Phi$  maps the tangent space at  $p_1$  to the tangent space at  $p_2$ , thus facilitating a comparison between  $\mathfrak{g}_{p_1}$  and  $\mathfrak{g}_{p_2}$ , which otherwise are defined on different domains. A body is materially uniform if a material isomorphism exists between any two points in the body. Moreover, for the existence of a material isomorphism, it is necessary that the response functional is not explicitly dependent on the material point (i.e.  $\mathfrak{g}_{p_1}$  can not be an explicit function of  $p_1$ ). This follows immediately

from the definition of material isomorphism above. Any two material isomorphisms are related by (equation (6.3) in [129])

$$\hat{\Phi} = \mathbf{G}\Phi\mathbf{G}^T, \quad (3.166)$$

where  $\mathbf{G}$  belongs to the isotropy group (or symmetry group) relative to the intermediate configuration. Recall from Section 3.6 that  $\mathbf{G}$  is uniform (that is, independent of the position). It has been shown by Noll [129] (equations (6.4) and (6.5)) that any material isomorphism can be represented as

$$\Phi(p_1, p_2) = \mathbf{K}^{-1}(p_1)\mathbf{K}(p_2). \quad (3.167)$$

Consider a second reference configuration  $\hat{\mathbf{K}}$  with material isomorphism given by (3.166). It then follows from (3.166) and (3.167) that

$$\hat{\mathbf{K}}(p_2)\mathbf{G}\mathbf{K}^{-1}(p_2) = \hat{\mathbf{K}}(p_1)\mathbf{G}\mathbf{K}^{-1}(p_1) = \mathbf{L}, \quad (3.168)$$

where  $\mathbf{L} \in Lin$  is uniform. Consequently, these two reference configurations can be related by

$$\hat{\mathbf{K}} = \mathbf{L}\mathbf{P}\mathbf{K}, \quad (3.169)$$

where

$$\mathbf{P}(p_1) = \mathbf{K}(p_1)\mathbf{G}^{-1}\mathbf{K}^{-1}(p_1) \quad (3.170)$$

belongs to the symmetry group relative to the reference configuration given by  $\mathbf{K}$ . This last claim follows from the relation (3.18).

Recall (3.25) and note that the transformation  $\mathbf{K} \rightarrow \hat{\mathbf{K}} = \mathbf{A}\mathbf{K}$  leaves the total dislocation density  $\alpha$  invariant only if  $\mathbf{A}$  is continuously differentiable and can be expressed as

a gradient (here,  $\mathbf{A}$  is identified with  $\mathbf{LP}$ , cf. (3.169)). In case of discrete symmetry groups, the tensor  $\mathbf{P}$  at two neighboring material points, if not identical, will be discontinuous. A nonuniform  $\mathbf{P}$  will consequently violate the continuity of  $\hat{\mathbf{K}}$ . Therefore, in order to have a smooth plastic distortion field (which is required to obtain  $\boldsymbol{\alpha}$ ),  $\mathbf{P}$  has to be uniform for a material with discrete symmetry group. As a result,  $\mathbf{A} = \mathbf{LP}$  is uniform, and therefore  $\boldsymbol{\alpha}$  remains invariant under compatible changes in the reference configuration. On the other hand, for continuous symmetry groups (e.g. isotropy and transverse isotropy), one can construct a smooth  $\mathbf{P}$  field which can not be expressed as a gradient. In such a situation, the total dislocation density is no more invariant, and therefore fails to be a genuine measure of incompatibility. This conclusion was reached by Noll [129] in theorem 8 of his mentioned paper. A further exposition was given by Cohen and Epstein [37], who also quantified the non-uniqueness introduced by the continuous symmetry groups.

We can therefore conclude that our model ceases to be valid, for bodies with continuous symmetry groups, such as isotropic or transversely isotropic symmetry. However, it should be noted that such continuous symmetries are, in practice, used to model polycrystals, which are random aggregates of single crystals and at sufficiently large scales, can be viewed as isotropic. To model a poly-crystalline material within our framework, we would need to construct the theory at the level of an individual grain boundary, which separates single crystals. This is precisely the aim of Chapter 6 in this thesis.

*Remark 3.8.4.* (Bauschinger effect) We observe that the present model, based on the idea of a stress-free manifold, does not admit *back stress* as a constitutive variable.<sup>19</sup> Back

---

<sup>19</sup>Gurtin [70, 71] derives a back stress from the dependence of energy on dislocation density, thus attributing the Bauschinger effect to the constitutive nature of a strain-gradient theory of plasticity.

stress is thought to be responsible for the Bauschinger effect [109]. Instead, back stress is regarded as residual stress arising from a dislocation density distribution and a consequent distribution of elastic strain. In principle, the residual stress field may be determined from the dislocation density distribution [93, 176] and is therefore a feature of the solution to a suitably posed initial-boundary-value problem. Its presence effectively means that the proximity of the local stress state to the yield manifold varies over the body, and thus that yield in a loaded body is non-uniformly distributed. From this point of view the Bauschinger effect is structural, rather than constitutive, in nature.



## Chapter 4

# Plasticity with Small Elastic Strains and Elastic Rigidity

In the previous chapter, except for our choice of state variables, the theory of elastic-plastic deformation was fairly general. In particular, no specific choice for flow rules and yield criteria were considered. The purpose of this brief chapter is to obtain more specific results under assumptions on the nature of plastic work and on the accompanying elastic deformation during the plastic flow. Moreover, we will be restricting ourselves to *isothermal* and *rate-independent* processes. We also emphasize how our model reduces to classical models of phenomenological plasticity. Some standard texts on plasticity theory should be mentioned here. The books by Hill [75], Bridgman [22], Kachanov [82], Prager and Hodge [145], and Thomas [165] are a few, which provide an excellent introduction to classical theories of plasticity.

This chapter is divided into three sections. We start with a postulate of Ilyushin,

according to which the plastic work is always non-negative for a process with coinciding initial and final deformation gradient fields. This postulate furnishes a sufficient condition for obtaining associated flow rules and a convex yield surface. In Section 4.2 we assume the elastic strain to be infinitesimally small, but still allowing for finite rotations and finite plastic strain. After reducing our general theory in the light of this assumption, we discuss, in detail, the nature of associated flow rules in the absence and presence of hardening. The last section is concerned with elastically rigid and perfectly plastic solids. For elastically rigid solids, the elastic strain is assumed to vanish completely, thereby reducing  $\mathbf{H}$  to a rotation. The stress  $\mathbf{S}$  is indeterminate in such a situation (since there is no strain energy), but it can be understood as the Lagrange multiplier associated with the constraint of imposing  $\mathbf{H}$  to be a rotation. The assumption of perfectly plastic behavior requires absence of any hardening in the model. Therefore our flow rules and yield criterion are independent of  $\alpha$ . The theory of elastically rigid perfectly plastic bodies is fundamentally different from what we have modeled so far, as the notion of stress is no longer constitutive and derived from an energy, but is rather of the nature of a Lagrange multiplier. Many of our conclusions in the previous chapter rest on the existence of a strain energy, and therefore it is important to revisit the theory when no strain energy can be assumed. Such is the aim of this last section, which is concluded with an example from the theory of Lüders bands [165] in the context of cubic symmetry.

## 4.1 Ilyushin's postulate

The concepts of associated flow rule and convex yield surface are central to many theories of rate-independent phenomenological plasticity. An associated flow rule is one for which the change in plastic distortion, which in our general representation of flow rules is given by  $\mathbf{K}^{-1}\dot{\mathbf{K}}$  (cf. (3.137)), is in the direction of the normal to the yield surface (a precise definition of this normal is given below). The flow rule is therefore *associated* with the yield criterion.

Various dissipation postulates have been proposed which provide sufficient conditions to derive an associated flow rule with a convex yield surface. The principle of maximum plastic dissipation (see for e.g. Hill [75], page 66) is one of the most used postulates, according to which plastic flow evolves so as to maximize the plastic work expended by the body. If taken independently, such a postulate has no physical motivation beyond its utility in proving certain existence and uniqueness theorems (see Chapter 3 of [75]). In the early 1950s, Drucker [43] introduced an inequality, which should be satisfied by all work hardening materials. According to Drucker's inequality, for a complete cycle of additional loading and unloading, additional stresses do positive work in the presence of plastic deformation. A consequence is that the plastic strain rate cannot oppose the stress rate (see §18 in [82] and Section 3.2 in [109] for details). The principle of maximum dissipation follows from Drucker's inequality and therefore its validity could be justified at least for the physical situations assumed by Drucker. However, Drucker's inequality ceases to be valid for finite elastic/plastic strains [79, 110] and for strain softening [109]. Motivated by this shortcoming, Ilyushin [80] proposed another condition which remains valid for finite elastic/plastic

strains and also for materials which exhibit strain softening [112, 109]. Ilyushin's postulate is equivalent to Drucker's postulate only for small elastic/plastic strains [110]. As shown below, the postulate of Ilyushin implies the principle of maximum dissipation.<sup>1</sup>

The thermodynamic state of an isothermal material element is given by  $\{\mathbf{F}, \mathbf{H}\}$  (cf. Subsection 3.4.1).<sup>2</sup> In the state space, we consider closed cycles for a time interval  $[t_1, t_2]$  (where  $t_2 > t_1$  and  $t_1, t_2 \in \mathbb{R}$ ), such that  $\mathbf{F}(t_1) = \mathbf{F}(t_2)$ . Moreover, assume that these closed cycles begin inside (or on) the yield surface (i.e.  $\mathbf{H}(t_1)$  is such that  $g \leq 0$  at  $t = t_1$ , cf. (3.163)). According to Ilyushin's postulate, for a closed cycle (in the sense defined above), the net work done (at a fixed material point) is non-negative. The work done at a fixed material point is given by  $\mathbf{P} \cdot \dot{\mathbf{F}}$ , cf. (2.168). We therefore have

$$\int_{t_1}^{t_2} \mathbf{P}(t) \cdot \dot{\mathbf{F}}(t) dt \geq 0. \quad (4.1)$$

Recalling (3.73) (with  $\dot{\theta} = 0$ ), we can rewrite the integrand in (4.1) as  $\mathbf{P} \cdot \dot{\mathbf{F}} = \rho_\kappa \dot{f} + \mathbf{E} \cdot \dot{\mathbf{K}} \mathbf{K}^{-1}$ , where  $\rho_\kappa f = J_K^{-1} W(\mathbf{H})$  is the strain energy per unit volume of the reference configuration and  $\mathbf{E} = J_K^{-1} W \mathbf{1} - \mathbf{F}^T \mathbf{P}$  is Eshelby's energy-momentum tensor. The inequality thus can be written as

$$\int_{t_1}^{t_2} (\rho_\kappa \dot{f} + \mathbf{E} \cdot \dot{\mathbf{K}} \mathbf{K}^{-1}) dt \geq 0. \quad (4.2)$$

Assume the plastic loading to take place for the time interval  $[t_a, t_b] \subset [t_1, t_2]$ , where  $t_b > t_a$  and  $t_a, t_b \in \mathbb{R}$ . Then  $\dot{\mathbf{K}} \neq \mathbf{0}$  only for time,  $t \in [t_a, t_b]$ . Moreover, note that  $\mathbf{K}(t_2) = \mathbf{K}(t_b)$

---

<sup>1</sup>The consequences of Ilyushin's postulate in the context of finite distortions have been investigated in [126, 107, 111, 112, 167, 157].

<sup>2</sup>We are therefore considering only those material points which are away from the singular surface. For material points on the singular surface, the state is otherwise given by  $\{\mathbf{F}^\pm, \mathbf{H}^\pm\}$ .

and  $\mathbf{K}(t_a) = \mathbf{K}(t_1)$ . The inequality (4.2) therefore reduces to

$$\rho_\kappa f(\mathbf{F}(t_2), \mathbf{K}(t_2)) - \rho_\kappa f(\mathbf{F}(t_1), \mathbf{K}(t_1)) + \int_{t_a}^{t_b} \mathbf{E} \cdot \dot{\mathbf{K}} \mathbf{K}^{-1} dt \geq 0 \quad (4.3)$$

or equivalently

$$\rho_\kappa f(\mathbf{F}(t_1), \mathbf{K}(t_b)) - \rho_\kappa f(\mathbf{F}(t_1), \mathbf{K}(t_a)) + \int_{t_a}^{t_b} \mathbf{E} \cdot \dot{\mathbf{K}} \mathbf{K}^{-1} dt \geq 0, \quad (4.4)$$

where we have also used the fact that  $\mathbf{F}(t_1) = \mathbf{F}(t_2)$ . Since  $f$  is differentiable with respect to  $\mathbf{K}$ , (4.4) furnishes

$$\int_{t_a}^{t_b} (\rho_\kappa f_{\mathbf{K}}(\mathbf{F}(t_1), \mathbf{K}) \cdot \dot{\mathbf{K}} + \mathbf{E} \cdot \dot{\mathbf{K}} \mathbf{K}^{-1}) dt \geq 0. \quad (4.5)$$

Use the mean value theorem, and then take the limit  $t_b \rightarrow t_a$  (after dividing the expression by  $t_b - t_a$ ) to obtain

$$(\rho_\kappa f_{\mathbf{K}}(\mathbf{F}(t_1), \mathbf{K}) \cdot \dot{\mathbf{K}} + \mathbf{E} \cdot \dot{\mathbf{K}} \mathbf{K}^{-1}) \geq 0, \quad (4.6)$$

evaluated at  $t = t_a$ . Now, use  $\rho_\kappa f(\mathbf{F}(t_1), \mathbf{K}(t)) = J_{\mathbf{K}(t)}^{-1} W(\mathbf{F}(t_1) \mathbf{K}(t))$  to obtain

$$\begin{aligned} \rho_\kappa f_{\mathbf{K}}(\mathbf{F}(t_1), \mathbf{K}(t)) &= -J_{\mathbf{K}(t)}^{-1} \mathbf{K}^{-T}(t) W(\mathbf{F}(t_1) \mathbf{K}(t)) - J_{\mathbf{K}(t)}^{-1} \mathbf{F}^T(t_1) W_{\mathbf{H}} \\ &= -\mathbf{E}(\mathbf{F}(t_1), \mathbf{K}(t)) \mathbf{K}^{-T}(t). \end{aligned} \quad (4.7)$$

Substitute this result into (4.6) to get

$$\{\mathbf{E}(\mathbf{F}(t), \mathbf{K}(t)) - \mathbf{E}(\mathbf{F}(t_1), \mathbf{K}(t))\} \cdot \dot{\mathbf{K}}(t) \mathbf{K}^{-1}(t) \geq 0, \quad (4.8)$$

which on using  $\mathbf{E} = J_{\mathbf{K}}^{-1} \mathbf{K}^{-T} \mathbf{E}' \mathbf{K}^T$ , where  $\mathbf{E}' = \hat{W}(\mathbf{C}_H) \mathbf{1} - \mathbf{C}_H \mathbf{S}(\mathbf{C}_H)$  and  $\mathbf{S} = 2Sym \hat{W}_{\mathbf{C}_H}$ , can be rewritten as

$$\{\mathbf{E}'(\mathbf{C}_H(t)) - \mathbf{E}'(\mathbf{C}_H(t_1))\} \cdot \mathbf{K}^{-1}(t) \dot{\mathbf{K}}(t) \geq 0. \quad (4.9)$$

Recall, that the dissipation (away from the singular surface) for an isothermal process was obtained to be (cf. (3.75), (3.78))

$$D = \mathbf{E} \cdot \dot{\mathbf{K}}\mathbf{K}^{-1} = J_K^{-1} \mathbf{E}' \cdot \mathbf{K}^{-1} \dot{\mathbf{K}}. \quad (4.10)$$

Moreover, our choice of state at  $t = t_1$  is arbitrary as long as  $g(t_1) \leq 0$ , where  $g = 0$  defines the yield surface. For fixed  $\mathbf{K}^{-1} \dot{\mathbf{K}}$ , the inequality (4.9) therefore restricts the state achieved by the material element to be the one which maximizes dissipation with respect to all the thermodynamic states on or inside the yield surface. A similar interpretation follows from (4.8). The inequalities (4.8) and (4.9) can be seen as two equivalent statements of the principle of maximum plastic dissipation. Note that, these inequalities are only necessary conditions for Ilyushin's postulate. Their sufficiency can be proved only under much restrictive conditions [112].

We now discuss the consequences of inequality (4.9). Assume the yield surface to be smooth everywhere and given by

$$G(\mathbf{E}', \boldsymbol{\alpha}) = 0, \quad (4.11)$$

such that  $g = \hat{g}(\mathbf{C}_H, \boldsymbol{\alpha}) = G(\mathbf{E}'(\mathbf{C}_H), \boldsymbol{\alpha})$  (cf. (3.163)). For fixed  $\boldsymbol{\alpha}$ ,  $\mathbf{E}'(\mathbf{C}_H(t))$  lies on the manifold  $G = 0$  and  $\hat{\mathbf{E}}' = \mathbf{E}'(\mathbf{C}_H(t_1))$  lies in the domain restricted by  $G \leq 0$  (see Figure 4.1). They are related via the inequality (4.9) as

$$(\mathbf{E}' - \hat{\mathbf{E}}') \cdot \mathbf{K}^{-1} \dot{\mathbf{K}} \geq 0. \quad (4.12)$$

We can use our constitutive assumptions to interpret second order tensors  $\mathbf{K}^{-1} \dot{\mathbf{K}}$ ,  $\mathbf{E}'$ , and  $\hat{\mathbf{E}}'$  as members of a six dimensional vector space. Indeed, recall our assumption regarding plastic spin from (3.134), i.e.  $\mathbf{K}^{-1} \dot{\mathbf{K}} \mathbf{C}_H^{-1} \in Sym$ . This constitutive assumption reduces

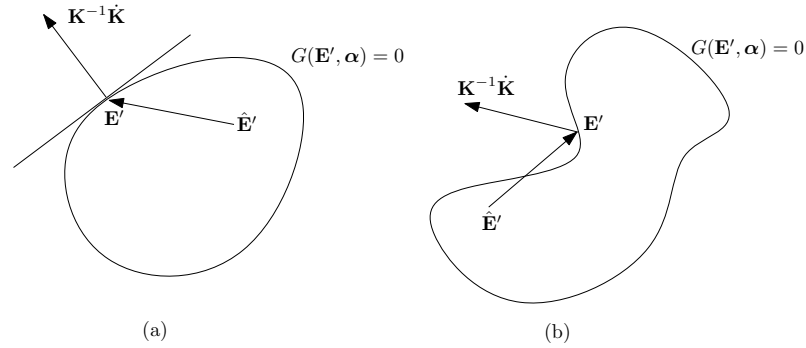


Figure 4.1: Associated flow rule and convexity of the yield surface.<sup>3</sup>

the number of unknown components in  $\mathbf{K}^{-1}\dot{\mathbf{K}}$  from nine to six. Furthermore, we have constraints of the form  $\mathbf{E}'\mathbf{C}_H \in Sym$  for  $\mathbf{E}'$ , thus reducing its dimension from nine to six. The surface  $G(\mathbf{E}', \alpha) = 0$  for a fixed  $\alpha$ , therefore represents a five dimensional manifold in the space of six dimensional vectors.

Interpreting the second order tensors  $\mathbf{K}^{-1}\dot{\mathbf{K}}$ ,  $\mathbf{E}'$ , and  $\hat{\mathbf{E}}'$  as six dimensional vectors, we can understand the inequality (4.12) as a requirement for the angle between  $(\mathbf{E}' - \hat{\mathbf{E}}')$  and  $\mathbf{K}^{-1}\dot{\mathbf{K}}$  to be acute. Assume that the surface  $G = 0$  is not convex (for example, as in Figure 4.1 (b)). Then it is always possible to choose a point  $\hat{\mathbf{E}}'$  such that the inequality (4.12) is violated, regardless of the direction of  $\mathbf{K}^{-1}\dot{\mathbf{K}}$ . Therefore the yield surface has to be convex. Referring now to Figure 4.1 (a), we can conclude that  $\mathbf{K}^{-1}\dot{\mathbf{K}}$  has to be in a direction of the outward normal (smoothness of  $G$  furnishes a unique normal) to the tangent hyperplane of  $G = 0$  at  $\mathbf{E}'$  (and at a fixed  $\alpha$ ). Otherwise, we can choose  $\mathbf{E}' - \hat{\mathbf{E}}'$  such that

---

<sup>3</sup>The yield surface  $G = 0$  represents a six dimensional manifold for fixed  $\alpha$ . The second order tensors  $\mathbf{K}^{-1}\dot{\mathbf{K}}$ ,  $\mathbf{E}'$ , and  $\hat{\mathbf{E}}'$  are all understood as members of a six dimensional vector space.

(4.12) is violated. This is the normality rule, which can be written as

$$\mathbf{K}^{-1}\dot{\mathbf{K}} = \mu G_{\mathbf{E}'}(\mathbf{E}', \boldsymbol{\alpha}), \quad (4.13)$$

where  $\mu \geq 0$  is a scalar multiplying factor. The non-negativity of  $\mu$  come from the fact that  $\mathbf{K}^{-1}\dot{\mathbf{K}}$  has to be an outward (and not inward) normal to  $G = 0$ . A more technical derivation, instead of purely geometric arguments used here, can be pursued using concepts from convex analysis.<sup>4</sup> Finally, note that the flow rule as obtained in (4.13) should also satisfy the following dissipation inequality (cf. (3.75) and (3.78) with  $\mathbf{g} = \mathbf{0}$ ), which follows as a consequence of the second law of thermodynamics:

$$\mathbf{E}' \cdot \mathbf{K}^{-1}\dot{\mathbf{K}} \geq 0. \quad (4.14)$$

Using (4.13), inequality (4.14) then yields (for  $\mu > 0$ )

$$\mathbf{E}' \cdot G_{\mathbf{E}'}(\mathbf{E}', \boldsymbol{\alpha}) \geq 0. \quad (4.15)$$

This inequality can be seen as a restriction on the form of the yield criteria  $G(\mathbf{E}', \boldsymbol{\alpha})$ .

*Remark 4.1.1.* (Plastic spin) If in the above discussion we remove the constraint on the plastic spin, given by  $\mathbf{K}^{-1}\dot{\mathbf{K}}\mathbf{C}_H^{-1} \in Sym$  (cf. (3.134)), then the relation (4.13) poses a problem. Without the constraint, the tensor  $\mathbf{K}^{-1}\dot{\mathbf{K}}$  belongs to a nine dimensional vector space, while on the other hand the right hand side of (4.13) lies in the local cotangent space of the  $\mathbf{E}'$  manifold, which is a six dimensional vector space. This issue was identified by Lubliner [108, 109] (and later by Cleja-Țigoiu [167]), who proposed a solution by adding to the right hand side of (4.13), a three dimensional vector orthogonal to  $G_{\mathbf{E}'}$  in the space

---

<sup>4</sup>See for example the derivation in Lucchesi and Podio-Guidugli [111], which relies heavily on the concepts introduced by Rockafellar [151].



of nine dimensional vectors, so as to make it consistent. We avoid this altogether by introducing an additional constitutive assumption on the nature of plastic spin.

*Remark 4.1.2.* (Yield surface in strain space) If the yield surface is given in terms of  $\mathbf{C}_H$  rather than  $\mathbf{E}'$ , then we would require to invert  $\mathbf{E}' = \mathbf{E}'(\mathbf{C}_H)$  to express the normality rule (4.13) in terms of the yield surface in strain space [167]. This in general is not valid in the case of finite elastic strains, due to non invertibility of the stress strain relation . However, as we shall see in the next section, this problem is overcome in the case of small elastic strains.

## 4.2 Small elastic strains

For many practical problems, specifically in the case of metals, elastic strains remain infinitesimally small and the material starts to flow plastically even under small strains. The rotation appearing in the polar decomposition of  $\mathbf{H}$  however can remain finite, a fact which has important implications for the magnitude of dislocation density. The plastic distortion also, in general, remains finite. It would be therefore interesting to simplify our theory under the assumption of infinitesimal elastic strain. A more restrictive assumption is of course of an absence of elastic strains. This assumption, however, requires us to approach the theory in a fundamentally different way, and not just as a limiting case. We will discuss the consequences of the assumption of elastic rigidity in Section 4.3.

### 4.2.1 Preliminaries

Denote the Elastic strain by  $\epsilon$  and assume it to be small, i.e.  $|\epsilon| \ll 1$ . The left Cauchy Green tensor  $\mathbf{C}_H = \mathbf{H}^T \mathbf{H}$  is related to the elastic strain as  $\mathbf{C}_H = 2\epsilon + \mathbf{1}$ . The elastic distortion  $\mathbf{H}$  admits a polar decomposition (cf. (2.35)), i.e.  $\mathbf{H} = \mathbf{R}\mathbf{U}$ , where  $\mathbf{R} \in Orth^+$  is a rotation and  $\mathbf{U} \in Sym^+$  is symmetric and positive definite. Since  $\mathbf{U}^2 = \mathbf{C}_H$ , we obtain  $\mathbf{U} = \mathbf{1} + \epsilon + o(|\epsilon|)$  and consequently

$$\mathbf{H} = \mathbf{R}(\mathbf{1} + \epsilon) + o(|\epsilon|), \quad \mathbf{H}^{-1} = (\mathbf{1} - \epsilon)\mathbf{R}^T + o(|\epsilon|), \quad \text{and } J_H = 1 + O(|\epsilon|). \quad (4.16)$$

Recall relations (3.100) and (3.101) for stresses. If we assume

$$\mathbf{S} = O(|\epsilon|) \quad (4.17)$$

such that  $\mathbf{S}$  vanishes for a zero elastic strain, then we can write the linear relationship between stress and strain as

$$\mathbf{S} = \mathbb{C}[\epsilon], \quad (4.18)$$

where  $\mathbb{C}$  is the fourth order constant elastic modulus tensor (see Page 22 for more on fourth order tensors). The tensor  $\mathbb{C}$  has a major symmetry and also minor symmetries with respect to first two and last two indices. The strain energy, then has the following form (assuming that there is zero strain energy in the absence of  $\epsilon$ )

$$W = \frac{1}{2} \mathbb{C}[\epsilon] \cdot \epsilon. \quad (4.19)$$

On the other hand, use (3.100), (4.16)<sub>1,3</sub>, and (4.17) to obtain an estimate for Cauchy stress,

$$\mathbf{T} = \mathbf{R}\mathbf{S}\mathbf{R}^T + o(|\epsilon|). \quad (4.20)$$

The Eshelby's tensor  $\mathbf{E}' = \hat{W}(\mathbf{C}_H)\mathbf{1} - \mathbf{C}_H\mathbf{S}(\mathbf{C}_H)$ , on using (4.17), (4.19), and  $\mathbf{C}_H = \mathbf{1} + 2\boldsymbol{\epsilon}$ , can be written as

$$\mathbf{E}' = -\mathbf{S} + o(|\boldsymbol{\epsilon}|). \quad (4.21)$$

The dissipation inequality (3.75) therefore takes the form

$$D \approx -\mathbf{S} \cdot \mathbf{K}^{-1}\dot{\mathbf{K}} = \mathbf{S} \cdot \mathbf{K}^{-1}\dot{\mathbf{K}} \geq 0, \quad (4.22)$$

where  $\mathbf{K}^{-1}$  represents the material time derivative of  $\mathbf{K}^{-1}$ . The second equality in (4.22) is obtained on using the identity,  $\mathbf{K}^{-1}\dot{\mathbf{K}} + \dot{\mathbf{K}}^{-1}\mathbf{K} = \mathbf{0}$ , which follows from taking the time derivative of  $\mathbf{K}^{-1}\mathbf{K} = \mathbf{1}$ . Moreover our constitutive assumption regarding plastic spin (3.134), to the leading order, is now give by

$$\mathbf{K}^{-1}\dot{\mathbf{K}} \in \text{Sym}. \quad (4.23)$$

Recall the flow rule (3.137),

$$\mathbf{K}^{-1}\dot{\mathbf{K}} = \mathcal{S}(\mathbf{C}_H, \dot{\mathbf{C}}_H, \boldsymbol{\alpha})\mathbf{C}_H, \quad (4.24)$$

where  $\mathcal{S} \in \text{Sym}$ . Use  $\mathbf{C}_H = \mathbf{1} + 2\boldsymbol{\epsilon}$  to define  $\hat{\mathcal{S}} \in \text{Sym}$  as  $\hat{\mathcal{S}}(\boldsymbol{\epsilon}, \dot{\boldsymbol{\epsilon}}, \boldsymbol{\alpha}) = \mathcal{S}(\mathbf{1} + 2\boldsymbol{\epsilon}, 2\dot{\boldsymbol{\epsilon}}, \boldsymbol{\alpha})$ .

Since  $\dot{\mathbf{K}}$  vanishes in the absence of elastic distortion (Section 3.5), we have  $\hat{\mathcal{S}}(\mathbf{0}, \dot{\boldsymbol{\epsilon}}, \boldsymbol{\alpha}) = \mathbf{0}$

by virtue of (3.137), and if  $\hat{\mathcal{S}}$  is a smooth function of its first argument, (4.24) furnishes

$$\mathbf{K}^{-1}\dot{\mathbf{K}} = \mathcal{T}(\boldsymbol{\epsilon}, \dot{\boldsymbol{\epsilon}}, \boldsymbol{\alpha}) + o(|\boldsymbol{\epsilon}|), \quad (4.25)$$

where  $\mathcal{T}(\boldsymbol{\epsilon}, \dot{\boldsymbol{\epsilon}}, \boldsymbol{\alpha})$  is a symmetric tensor valued function *linear* in  $\boldsymbol{\epsilon}$ . In the rate-independent case it is also linear in  $\dot{\boldsymbol{\epsilon}}$ . Given the one-to-one relationship between  $\mathbf{S}$  and  $\boldsymbol{\epsilon}$  implied by our constitutive assumptions, we may write

$$\mathbf{K}^{-1}\dot{\mathbf{K}} = \mathcal{R}(\mathbf{S}, \dot{\mathbf{S}}, \boldsymbol{\alpha}) + o(|\mathbf{S}|), \quad (4.26)$$

in which  $\mathbf{S}$  is non-dimensionalized by the largest modulus in the linear function  $\mathbf{S}(\boldsymbol{\epsilon})$ , and  $\mathcal{R}(\mathbf{S}, \dot{\mathbf{S}}, \boldsymbol{\alpha}) = \mathcal{T}(\boldsymbol{\epsilon}(\mathbf{S}), (\dot{\boldsymbol{\epsilon}}(\mathbf{S})), \boldsymbol{\alpha})$  is a symmetric tensor valued function linear in  $\mathbf{S}$  (and also in  $\dot{\mathbf{S}}$  in the rate-independent case). Substitute (4.26) into (4.22) yields

$$\mathbf{S} \cdot \mathcal{R}(\mathbf{S}, \dot{\mathbf{S}}, \boldsymbol{\alpha}) \leq 0, \quad (4.27)$$

with equality holding only when  $\dot{\mathbf{K}} = \mathbf{0}$ . Further, since, under material symmetry,  $\boldsymbol{\epsilon}$  and  $\mathbf{S}$  transform to  $\mathbf{G}^T \boldsymbol{\epsilon} \mathbf{G}$  and  $\mathbf{G}^T \mathbf{S} \mathbf{G}$ , respectively (where  $\mathbf{G}$  belongs to the symmetry group  $\mathcal{G}_{\kappa_i}$  associated with  $\kappa_i$ ), the representation problems for  $\mathcal{T}(\boldsymbol{\epsilon}, \dot{\boldsymbol{\epsilon}}, \boldsymbol{\alpha})$  and  $\mathcal{R}(\mathbf{S}, \dot{\mathbf{S}}, \boldsymbol{\alpha})$  are the same as that for  $\mathcal{S}$ , except of course that the former are eased considerably by the linear dependence on the first arguments, or by the bilinear dependence on the first two arguments in the case of rate independence.

In the same way, if the yield function  $g$  (cf. (3.163)) depends smoothly on its first argument, then

$$g(\mathbf{C}_H, \boldsymbol{\alpha}) = H(\boldsymbol{\epsilon}, \boldsymbol{\alpha}) + o(|\boldsymbol{\epsilon}|^2), \quad (4.28)$$

where  $H$  contains terms linear and quadratic in  $\boldsymbol{\epsilon}$ . Our constitutive hypothesis imply that this may be written as a similar function of  $\mathbf{S}$ . Denote such a function by  $\tilde{H}(\mathbf{S}, \boldsymbol{\alpha}) = H(\boldsymbol{\epsilon}, \boldsymbol{\alpha})$ . These functions are subject to material symmetry restrictions which follow trivially from (3.164). Taylor's formula for the flow stress in single crystals involves a linear relationship between the square of stress and the operative dislocation density. This suggests that a linear dependence of  $H$  on  $\boldsymbol{\alpha}$  is relevant. Yield functions of this kind (modulo dislocation density) have recently been studied [28] and correlated with experimental data on materials having various kinds of symmetry. These may be adapted directly to the present framework by using  $\mathbf{S}$  as the operative stress measure and regarding  $\mathcal{G}_{\kappa_i}$  as the relevant symmetry group.

### 4.2.2 Associated flow rules

For small elastic strains, relation (4.12) on using (4.21), reduces to

$$(\mathbf{S} - \hat{\mathbf{S}}) \cdot \dot{\mathbf{K}}^{-1} \mathbf{K} \geq 0, \quad (4.29)$$

where  $\hat{\mathbf{S}}$  is any stress satisfying  $\tilde{H}(\hat{\mathbf{S}}, \boldsymbol{\alpha}) \leq 0$  and  $\mathbf{S}$  is the stress which is truly achieved during plastic flow. On noting the definition of dissipation from (4.22), the inequality (4.29), as in Section 4.1, represents the principle of maximum dissipation. Following the arguments from Section 4.1, we can express the plastic evolution using an associated flow rule as<sup>5</sup>

$$\dot{\mathbf{K}}^{-1} \mathbf{K} = \lambda \tilde{H}_{\mathbf{S}}, \quad (4.30)$$

where  $\lambda \geq 0$  is a scalar. The second order tensors  $\dot{\mathbf{K}}^{-1} \mathbf{K}$  and  $\mathbf{S}$  can be identified with the six dimensional vector space of symmetric tensors. The yield criterion  $\tilde{H}(\mathbf{S}, \boldsymbol{\alpha}) = 0$ , for a fixed  $\boldsymbol{\alpha}$ , then defines a five dimensional manifold in this six dimensional vector space. Note that in the previous section, the six dimensional vector space did not correspond to the space of symmetric tensors.

To establish the transformation of  $\tilde{H}_{\mathbf{S}}$  under material symmetry, write a relation of the type (3.164) for  $\tilde{H}$

$$\tilde{H}(\mathbf{S}, \boldsymbol{\alpha}) = \tilde{H}(\mathbf{G}^T \mathbf{S} \mathbf{G}, \mathbf{G}^T \boldsymbol{\alpha} \mathbf{G}), \quad (4.31)$$

where  $\mathbf{G} \in \mathcal{G}_{\kappa_i}$  is a rotation. Fix  $\mathbf{G}$ , and take a time derivative of (4.31) to get

$$\tilde{H}_{\mathbf{S}} \cdot \dot{\mathbf{S}} + \tilde{H}_{\boldsymbol{\alpha}} \cdot \dot{\boldsymbol{\alpha}} = \mathbf{G} \tilde{H}_{\mathbf{S}} \mathbf{G}^T \cdot \dot{\mathbf{S}} + \mathbf{G} \tilde{H}_{\boldsymbol{\alpha}} \mathbf{G}^T \cdot \dot{\boldsymbol{\alpha}}, \quad (4.32)$$

---

<sup>5</sup>The gradient  $\tilde{H}_{\mathbf{S}}$  is a symmetric tensor, cf. the footnote on Page 79.

where  $\bar{\mathbf{S}} = \mathbf{G}^T \mathbf{S} \mathbf{G}$  and  $\bar{\boldsymbol{\alpha}} = \mathbf{G}^T \boldsymbol{\alpha} \mathbf{G}$ . Matching coefficients of  $\dot{\mathbf{S}}$  and  $\dot{\boldsymbol{\alpha}}$ , we get the transformations for  $\tilde{H}_{\mathbf{S}}$  and  $\tilde{H}_{\boldsymbol{\alpha}}$  as

$$\tilde{H}_{\bar{\mathbf{S}}} = \mathbf{G}^T \tilde{H}_{\mathbf{S}} \mathbf{G}, \quad \text{and} \quad \tilde{H}_{\bar{\boldsymbol{\alpha}}} = \mathbf{G}^T \tilde{H}_{\boldsymbol{\alpha}} \mathbf{G}, \quad (4.33)$$

respectively. Further, the invariance of  $\lambda$  follows from noting that  $\mathbf{K}^{-1} \dot{\mathbf{K}} \rightarrow \mathbf{G}^T \mathbf{K}^{-1} \dot{\mathbf{K}} \mathbf{G}$  (cf. (3.140)) and the transformation (4.33)<sub>1</sub>.

We now recover some classical flow rules. Use  $\mathbf{F} = \mathbf{H} \mathbf{K}^{-1}$  (cf. (3.18)) to obtain

$$\dot{\mathbf{F}} \mathbf{F}^{-1} = \dot{\mathbf{H}} \mathbf{H}^{-1} + \mathbf{H} \mathbf{K}^{-1} \dot{\mathbf{K}} \mathbf{H}^{-1}. \quad (4.34)$$

Here,  $\dot{\mathbf{H}} \mathbf{H}^{-1} = \dot{\mathbf{R}} \mathbf{R}^T + \mathbf{R} \dot{\boldsymbol{\epsilon}} \mathbf{R}^T + o(|\boldsymbol{\epsilon}|)$ , which follows from (4.16)<sub>1,2</sub> and the assumption that  $\dot{\boldsymbol{\epsilon}} = O(|\boldsymbol{\epsilon}|)$ . Moreover, assume  $\lambda = O(1)$  and  $\tilde{H}_{\mathbf{S}} = O(|\boldsymbol{\epsilon}|)$ . Then (4.30) when combined with (4.16)<sub>1,2</sub> furnishes

$$\mathbf{H} \mathbf{K}^{-1} \dot{\mathbf{K}} \mathbf{H}^{-1} = \lambda \mathbf{R} \tilde{H}_{\mathbf{S}} \mathbf{R}^T + o(|\boldsymbol{\epsilon}|). \quad (4.35)$$

The rate of deformation tensor  $\mathbf{D}$  is defined by  $\mathbf{D} = \text{Sym}(\dot{\mathbf{F}} \mathbf{F}^{-1})$ . Noting that  $\dot{\mathbf{R}} \mathbf{R}^T \in \text{Skw}$  and  $\tilde{H}_{\mathbf{S}} \in \text{Sym}$  we can obtain

$$\mathbf{D} = \mathbf{R} \dot{\boldsymbol{\epsilon}} \mathbf{R}^T + \lambda \mathbf{R} \tilde{H}_{\mathbf{S}} \mathbf{R}^T + o(|\boldsymbol{\epsilon}|). \quad (4.36)$$

For isotropy, relations (4.31) and (4.33) hold for all  $\mathbf{G} \in \text{Orth}^+$ . For  $\mathbf{G} = \mathbf{R}^T$ , we have  $\bar{\mathbf{S}} = \mathbf{G}^T \mathbf{S} \mathbf{G} = \mathbf{R} \mathbf{S} \mathbf{R}^T$  and therefore  $\bar{\mathbf{S}} \approx \mathbf{T}$  (cf. (4.20)). As a result

$$\tilde{H}_{\mathbf{T}} \approx \tilde{H}_{\bar{\mathbf{S}}} \approx \mathbf{R} \tilde{H}_{\mathbf{S}} \mathbf{R}^T, \quad (4.37)$$

where (4.37)<sub>2</sub> follows from (4.33)<sub>1</sub>. Substituting (4.37) back into (4.36) we get

$$\mathbf{D} \approx \mathbf{R} \dot{\boldsymbol{\epsilon}} \mathbf{R}^T + \lambda \tilde{H}_{\mathbf{T}}. \quad (4.38)$$

This is of the form of Prandtl–Reuss equation for plastic flow [82]. If additionally we assume that  $\dot{\boldsymbol{\epsilon}} = o(|\boldsymbol{\epsilon}|)$ , then  $\mathbf{D} \approx \lambda \tilde{H}_{\mathbf{T}}$ , which is the the classical Levy–St. Venant flow rule rule [82].

In the rest of this section, we will discuss the procedure to evaluate  $\lambda$ , which has been left undetermined so far. Significantly different results are obtained for the case of perfect plasticity (no hardening) and for a flow with hardening. We therefore divide the discussion into two parts:

**Case (i): No Hardening** Consider the case of perfect plasticity, that is plastic flow with no hardening. In our context this implies an absence of the dependence of flow rules and yield on  $\boldsymbol{\alpha}$ . The yield criterion is now given by

$$\tilde{H}(\mathbf{S}) = 0. \quad (4.39)$$

Using this yield criterion, we can obtain the consistency condition as

$$\tilde{H}_{\mathbf{S}} \cdot \dot{\mathbf{S}} = 0, \quad (4.40)$$

which can be rewritten in the form

$$\mathbf{HC}[\tilde{H}_{\mathbf{S}}] \cdot \dot{\mathbf{H}} = 0, \quad (4.41)$$

where we have used equation (4.18) and relations  $2\dot{\boldsymbol{\epsilon}} = \dot{\mathbf{C}}_H$ ,  $\tilde{H}_{\mathbf{S}} \in Sym$ , and  $\mathbb{C}^{\mathbb{T}} = \mathbb{C}$ . The superscript  $\mathbb{T}$  denotes the major transposition of a fourth order tensor (defined on page 22).

Since  $\mathbf{H} = \mathbf{FK}$ , (4.41) yields

$$\mathbf{HC}[\tilde{H}_{\mathbf{S}}] \cdot (\dot{\mathbf{F}}\mathbf{K} + \mathbf{F}\dot{\mathbf{K}}) = 0, \quad (4.42)$$

which can be rearranged, on using  $\mathbf{F} = \mathbf{H}\mathbf{K}^{-1}$  and  $\mathbf{K}^{-1}\dot{\mathbf{K}} = -\dot{\mathbf{K}}^{-1}\mathbf{K}$ , to get

$$\mathbf{H}\mathbf{C}[\tilde{\mathbf{H}}_{\mathbf{S}}]\mathbf{K}^T \cdot \dot{\mathbf{F}} - \mathbf{C}_H\mathbf{C}[\tilde{\mathbf{H}}_{\mathbf{S}}] \cdot \mathbf{K}^{-1}\dot{\mathbf{K}} = 0, \quad (4.43)$$

Substitute  $\mathbf{K}^{-1}\dot{\mathbf{K}}$  from the flow rule (4.30) into (4.43) and use the small strain approximation to obtain

$$\lambda = \frac{\mathbf{H}\mathbf{C}[\tilde{\mathbf{H}}_{\mathbf{S}}]\mathbf{K}^T \cdot \dot{\mathbf{F}}}{\mathbf{C}_H\mathbf{C}[\tilde{\mathbf{H}}_{\mathbf{S}}] \cdot \tilde{\mathbf{H}}_{\mathbf{S}}} \approx \frac{\mathbf{R}\mathbf{C}[\tilde{\mathbf{H}}_{\mathbf{S}}]\mathbf{K}^T \cdot \dot{\mathbf{F}}}{\mathbf{C}[\tilde{\mathbf{H}}_{\mathbf{S}}] \cdot \tilde{\mathbf{H}}_{\mathbf{S}}}, \quad (4.44)$$

where the denominator is assumed to be positive. Eliminating  $\lambda$  between (4.30) and (4.44) yields

$$\mathbf{K}^{-1}\dot{\mathbf{K}} = \phi(\tilde{\mathbf{H}}_{\mathbf{S}} \otimes \mathbf{R}\mathbf{C}[\tilde{\mathbf{H}}_{\mathbf{S}}]\mathbf{K}^T)\dot{\mathbf{F}}, \quad (4.45)$$

where

$$\phi = \frac{1}{\mathbf{C}[\tilde{\mathbf{H}}_{\mathbf{S}}] \cdot \tilde{\mathbf{H}}_{\mathbf{S}}}. \quad (4.46)$$

Similar results can be found in many texts of plasticity theory, for e.g. [75, 82].

**Case (ii): Hardening** For a model with hardening, the yield function depends on  $\boldsymbol{\alpha}$  and the yield criterion is given by

$$\tilde{H}(\mathbf{S}, \boldsymbol{\alpha}) = 0, \quad (4.47)$$

which then implies the following consistency condition

$$\tilde{H}_{\mathbf{S}} \cdot \dot{\mathbf{S}} + \tilde{H}_{\boldsymbol{\alpha}} \cdot \dot{\boldsymbol{\alpha}} = 0. \quad (4.48)$$

Our aim is to solve for  $\lambda$  which appears in the flow rule (4.30). In most of the conventional treatments [109], a separate flow rule is postulated for the hardening parameter, which in our case is  $\boldsymbol{\alpha}$ . In the following, however, we will use the definition of  $\boldsymbol{\alpha}$  from (3.23)<sub>1</sub> and obtain a partial differential equation to be solved for  $\lambda$ . This approach avoids



requiring additional constitutive information, which would be needed to postulate an independent flow rule for  $\dot{\boldsymbol{\alpha}}$ , at the cost of solving a differential equation for a scalar quantity. To elaborate, start by evaluating  $\dot{\boldsymbol{\alpha}}$  by taking the time derivative of the expression for  $\boldsymbol{\alpha}$  in (3.23)<sub>1</sub>. We get

$$\dot{\boldsymbol{\alpha}} = -\text{tr}(\dot{\mathbf{K}}^{-1}\mathbf{K})\boldsymbol{\alpha} + (\dot{\mathbf{K}}^{-1}\mathbf{K})\boldsymbol{\alpha} + J_K\mathbf{K}^{-1}\text{Curl}\dot{\mathbf{K}}^{-1}. \quad (4.49)$$

The term  $\dot{\mathbf{K}}^{-1}\mathbf{K}$  can be substituted directly from (4.30). On the other hand, the last term in (4.49) can be expanded using  $\dot{\mathbf{K}}^{-1} = \lambda\tilde{H}_S\mathbf{K}^{-1}$  (from (4.30)) as<sup>6</sup>

$$\begin{aligned} (\text{Curl}\dot{\mathbf{K}}^{-1})_{ij} &= e_{imn}(\lambda\tilde{H}_S\mathbf{K}^{-1})_{jn,m} \\ &= e_{imn}\lambda_{,m}(\tilde{H}_S\mathbf{K}^{-1})_{jn} + \lambda e_{imn}(\tilde{H}_S)_{jl,m}\mathbf{K}_{ln}^{-1} + \lambda(\tilde{H}_S)_{jl}(\text{Curl}\mathbf{K}^{-1})_{il}, \end{aligned}$$

which, when substituted back into (4.49), yields

$$\begin{aligned} \dot{\alpha}_{pj} &= \lambda\left((\tilde{H}_S)_{pk} - \text{tr}(\tilde{H}_S)\delta_{pk}\right)\alpha_{kj} + \lambda J_K e_{imn}K_{pi}^{-1}(\tilde{H}_S)_{jl,m}\mathbf{K}_{ln}^{-1} \\ &\quad + \lambda(\tilde{H}_S)_{jk}\alpha_{pk} + \lambda_{,m}J_K e_{imn}K_{pi}^{-1}(\tilde{H}_S\mathbf{K}^{-1})_{jn} \end{aligned} \quad (4.50)$$

and therefore

$$\begin{aligned} \tilde{H}\boldsymbol{\alpha} \cdot \dot{\boldsymbol{\alpha}} &= \lambda\left(\tilde{H}\boldsymbol{\alpha}\tilde{H}_S + \tilde{H}_S\tilde{H}\boldsymbol{\alpha}\right) \cdot \boldsymbol{\alpha} - \lambda\text{tr}(\tilde{H}_S)(\tilde{H}\boldsymbol{\alpha} \cdot \boldsymbol{\alpha}) \\ &\quad + \lambda J_K e_{imn}(\mathbf{K}^{-T}\tilde{H}\boldsymbol{\alpha})_{ij}(\tilde{H}_S)_{jl,m}\mathbf{K}_{ln}^{-1} + \lambda_{,m}J_K e_{imn}(\mathbf{K}^{-T}\tilde{H}\boldsymbol{\alpha}\tilde{H}_S\mathbf{K}^{-1})_{in}. \end{aligned} \quad (4.51)$$

On substituting (4.51) in the consistency condition (4.48), we obtain a partial differential equation (in space) to solve for  $\lambda$ . We note, simply by observation, that if the term  $\tilde{H}\boldsymbol{\alpha}$

---

<sup>6</sup>Indicial notation is used for simplicity. The components are with respect to the Cartesian coordinate system.

is volumetric (i.e. of the form  $a\mathbf{1}$ , for some  $a \in \mathbb{R}$ ), then the coefficient of  $\nabla\lambda$  in (4.51) vanishes, thereby reducing the differential equation to a linear equation in  $\lambda$ .

It will be useful, for use in Chapter 5, to express the flow rule (4.30) as a linear function of  $\dot{\mathbf{C}}_H$ . According to our constitutive assumptions  $\lambda$  in (4.30) should be a linear function of  $\dot{\mathbf{C}}_H$  (cf. (4.26)) and therefore can be written as

$$\lambda = \mathbf{M} \cdot \dot{\mathbf{C}}_H, \quad (4.52)$$

where  $\mathbf{M} = \mathbf{M}(\mathbf{C}_H, \boldsymbol{\alpha})$  is a symmetric second order tensor. The expression for  $\mathbf{M}$  can be obtained from (4.48) as

$$\mathbf{M} = -\frac{\lambda}{2} \frac{\mathbb{C}[\tilde{H}_{\mathbf{S}}]}{\tilde{H}_{\boldsymbol{\alpha}} \cdot \dot{\boldsymbol{\alpha}}}, \quad (4.53)$$

where we have also used  $\dot{\mathbf{S}} = \frac{1}{2}\mathbb{C}[\dot{\mathbf{C}}_H]$ , which follows from (4.18). We can verify (4.53) by a direct substitution into (4.52) and using (4.48). Rewrite (4.53) in the form

$$\mathbf{M} = \eta \mathbb{C}[\tilde{H}_{\mathbf{S}}], \quad (4.54)$$

with

$$\eta = -\frac{\lambda}{2\tilde{H}_{\boldsymbol{\alpha}} \cdot \dot{\boldsymbol{\alpha}}}, \quad (4.55)$$

where the denominator can be evaluated from (4.51). Use (4.54) and (4.52) to write the flow rule (4.30) as

$$\mathbf{K}^{-1}\dot{\mathbf{K}} = \eta \left( \tilde{H}_{\mathbf{S}} \otimes \mathbb{C}[\tilde{H}_{\mathbf{S}}] \right) [\dot{\mathbf{C}}_H]. \quad (4.56)$$

During plastic flow,  $\lambda > 0$  and  $\tilde{H}_{\mathbf{S}} \cdot \dot{\mathbf{S}} > 0$ . Therefore,  $\tilde{H}_{\boldsymbol{\alpha}} \cdot \dot{\boldsymbol{\alpha}} < 0$  (cf. (4.48)) and consequently (4.55) implies that  $\eta > 0$ .

### 4.3 Elastically rigid, perfectly plastic material

In this section, we assume our body to be elastically rigid and perfectly plastic, and restrict processes to be isothermal. An elastically rigid body is *not* capable of straining elastically (i.e.  $\epsilon = \mathbf{0}$  identically for all processes), and therefore, in the isothermal case, is unable to store any strain energy. Consequently, stress in the body is no longer derived from a strain energy. It can however be interpreted as the Lagrange multiplier associated with the constraint of elastic rigidity. On the other hand, the assumption of perfect plasticity requires the flow rule and the yield stress to be independent of any hardening parameter, which in our model is the dislocation density  $\alpha$ . There is a broad class of materials, which satisfy these assumptions [145, 75], and moreover, the resulting theory is analytically tractable to the extent of obtaining many closed form solutions [145].

Due to the nature of stress, the treatment of elastically rigid bodies proceeds in a fundamentally different way from the theory developed in Chapter 3, although much of the framework can be borrowed from it. In the first subsection below, we revisit main concepts developed in Chapter 3 in the light of present assumptions. In Subsection 4.3.2 we consider specific forms of yield functions and flow rules for the case of cubic material symmetry and use them in Subsection 4.3.3 to solve a problem involving Lüders bands.

#### 4.3.1 Preliminaries

For an elastic rigid body, the elastic distortion is given by a rotation. Such a constraint is expressed by six equations, and the corresponding Lagrange multipliers are the components of the symmetric Cauchy stress tensor. As before, the elastic deformation

and the Cauchy stress tensor are denoted by  $\mathbf{H} \in Orth^+$  and  $\mathbf{T} \in Sym$ , respectively.

**Relaxed configuration** It can be easily seen that two relaxed configurations (intermediate configurations) are locally related by a proper orthogonal tensor. Let  $\mathbf{H}_1$  and  $\mathbf{H}_2$  be the gradient of maps of the two relaxed configurations to the current configuration  $\kappa_t$  at a material point. If  $\mathbf{A}$  denotes the gradient of the map connecting the two relaxed configurations, then we can write,  $\mathbf{H}_1 = \mathbf{H}_2\mathbf{A}$ . For an elastically rigid body,  $\{\mathbf{H}_1, \mathbf{H}_2\} \in Orth^+$ , and therefore it follows immediately that  $\mathbf{A} \in Orth^+$ .

**Dissipation hypothesis** The multiplicative rule of decomposition for the deformation gradient  $\mathbf{F}$  yields  $\mathbf{H} = \mathbf{F}\mathbf{K}$  (cf. (3.18)), where  $\mathbf{K}$  denotes the plastic distortion. The stress power is given by  $\mathbf{P} \cdot \dot{\mathbf{F}}$ , where  $\mathbf{P} = J_F \mathbf{T}\mathbf{F}^{-T} = J_K^{-1} \mathbf{T}\mathbf{H}\mathbf{K}^T$  for  $\mathbf{H} \in Orth^+$ . For an elastically rigid solid, all the work done by stress is dissipated (since we assume storage of energy only through elastic strains). Thus, dissipation equals the stress power, i.e.  $D = \mathbf{P} \cdot \dot{\mathbf{F}}$ . Noting that  $\dot{\mathbf{F}} = \dot{\mathbf{H}}\mathbf{K}^{-1} - \mathbf{F}\dot{\mathbf{K}}\mathbf{K}^{-1}$ , and denoting  $\dot{\mathbf{H}}\mathbf{H}^{-1} = \Omega \in Skw$ , we can obtain  $D = \mathbf{P}\mathbf{F}^T \cdot \Omega - \mathbf{F}^T\mathbf{P} \cdot \dot{\mathbf{K}}\mathbf{K}^{-1}$ . But, since  $\mathbf{P}\mathbf{F}^T \in Sym$  (cf. (2.153)), we get  $D = -\mathbf{F}^T\mathbf{P} \cdot \dot{\mathbf{K}}\mathbf{K}^{-1}$ . We introduce the following dissipation hypothesis (cf. (3.87)):

$$D > 0 \text{ if and only if } \dot{\mathbf{K}} \neq \mathbf{0}, \text{ or}$$

$$\mathbf{F}^T\mathbf{P} \cdot \dot{\mathbf{K}}\mathbf{K}^{-1} < 0 \text{ if and only if } \dot{\mathbf{K}} \neq \mathbf{0}. \quad (4.57)$$

**Superimposed rigid body motion** We now obtain transformation rules for  $\mathbf{H}$  and  $\mathbf{K}$  under superimposed rigid body motions (SRBM). Let the elastic distortions associated with two such motions,  $\mathbf{H}_1$  and  $\mathbf{H}_2$ , be related by  $\mathbf{Z} = \mathbf{H}_2\mathbf{H}_1^{-1}$ . Since  $\{\mathbf{H}_1, \mathbf{H}_2\} \in Orth^+$ , therefore  $\mathbf{Z} \in Orth^+$ . Therefore under SRBM,  $\mathbf{H} \rightarrow \mathbf{Q}_H\mathbf{H}$ , where  $\mathbf{Q}_H \in Orth^+$ . To obtain

the transformation rule for  $\mathbf{K}$ , we introduce the hypothesis that SRBM does not generate dissipation. We also use the transformation rules for the deformation gradient and the Cauchy stress, i.e.  $\mathbf{F} \rightarrow \mathbf{Q}\mathbf{F}$  and  $\mathbf{T} \rightarrow \mathbf{Q}\mathbf{T}\mathbf{Q}^T$ , where  $\mathbf{Q} \in Orth^+$  denotes the rotation involved in the rigid body motion. Using the transformation rules for  $\mathbf{F}$  and  $\mathbf{H}$ , it is easily seen that  $J_K$  remains invariant. On using the transformation rule for  $\mathbf{T}$ , the term  $\mathbf{F}^T\mathbf{P}$  is found to be invariant under SRBM. Let  $\mathbf{Z} = \mathbf{K}_2\mathbf{K}_1^{-1}$ , with  $\mathbf{Z}(t_0) = \mathbf{I}$ , where  $t_0$  is the initial time of the rigid body motion. Let  $D_1$  and  $D_2$  denote the dissipation associated with  $\mathbf{K}_1$  and  $\mathbf{K}_2$  respectively. The above mentioned hypothesis then implies that

$$0 = D_1 - D_2 = \mathbf{F}_2^T\mathbf{P}_2 \cdot (\mathbf{K}_1^{-1}\dot{\mathbf{K}}_1 - \mathbf{K}_2^{-1}\dot{\mathbf{K}}_2), \quad (4.58)$$

which furnishes

$$\mathbf{F}_2^T\mathbf{P}_2 \cdot (\mathbf{K}_1^{-1}\mathbf{Z}^{-1}\dot{\mathbf{Z}}\mathbf{K}_1) = 0. \quad (4.59)$$

To obtain a necessary condition, let  $\mathbf{K}_1 = \mathbf{I}$ . The above condition then reduces to  $\mathbf{F}_2^T\mathbf{P}_2 \cdot (\mathbf{Z}^{-1}\dot{\mathbf{Z}}) = 0$ . Noting that  $\mathbf{K}_2 = \mathbf{Z}$ , we can invoke the hypothesis given by the relation (4.57) to conclude that  $\dot{\mathbf{Z}} = \mathbf{0}$  and therefore  $\mathbf{Z}(t) = \mathbf{Z}(t_0) = \mathbf{I}$ . Therefore under a SRBM,  $\mathbf{K} \rightarrow \mathbf{K}$ . The multiplicative decomposition of  $\mathbf{F}$ , then implies that  $\mathbf{Q}_H = \mathbf{Q}$ .

**Flow rule** In view of the dissipation inequality, the general form of flow rule can be written as

$$\mathcal{F}(\mathbf{K}, \dot{\mathbf{K}}, \mathbf{H}, \dot{\mathbf{H}}, \mathbf{F}^T\mathbf{P}, (\mathbf{F}^T\mathbf{P})) = \mathbf{0}, \quad (4.60)$$

where we have assumed the work hardening to be negligible in accordance with our assumption of perfect plasticity. We require the flow rule to be invariant under a compatible change in the reference configuration. Let  $\mathbf{R}$  be the gradient of the map connecting two reference

configurations  $\kappa_{r_1}$  and  $\kappa_{r_2}$ . Then  $\mathbf{F}_1 = \mathbf{F}_2\mathbf{R}$ ,  $\mathbf{H}_1 = \mathbf{H}_2$ , and  $\mathbf{K}_2 = \mathbf{R}\mathbf{K}_1$ . The Cauchy stress is insensitive to such changes in the reference configuration, and therefore  $\mathbf{P}_2 = J_R^{-1}\mathbf{P}_1\mathbf{R}^T$ . Insensitivity of the flow rule to a change in reference configuration then implies

$$\begin{aligned} & \mathcal{F}(\mathbf{K}_1, \dot{\mathbf{K}}_1, \mathbf{H}_1, \dot{\mathbf{H}}_1, \mathbf{F}_1^T\mathbf{P}_1, (\mathbf{F}_1^T\mathbf{P}_1)) \\ &= \mathcal{F}(\mathbf{R}\mathbf{K}_1, \mathbf{R}\dot{\mathbf{K}}_1, \mathbf{H}_1, \dot{\mathbf{H}}_1, J_R^{-1}\mathbf{R}^{-T}\mathbf{F}_1^T\mathbf{P}_1\mathbf{R}^T, J_R^{-1}\mathbf{R}^{-T}(\mathbf{F}_1^T\mathbf{P}_1)\mathbf{R}^T), \end{aligned} \quad (4.61)$$

where we have used the fact that  $\mathbf{R}$  is independent of time. Let  $\mathbf{R} = \mathbf{K}_1^{-1}$ , and obtain from (4.61),

$$\mathcal{F}(\mathbf{K}, \dot{\mathbf{K}}, \mathbf{H}, \dot{\mathbf{H}}, \mathbf{F}^T\mathbf{P}, (\mathbf{F}^T\mathbf{P})) = \hat{\mathcal{F}}(\mathbf{K}^{-1}\dot{\mathbf{K}}, \mathbf{H}, \dot{\mathbf{H}}, J_K\mathbf{K}^T\mathbf{F}^T\mathbf{P}\mathbf{K}^{-T}, J_K\mathbf{K}^T(\mathbf{F}^T\mathbf{P})\mathbf{K}^{-T}). \quad (4.62)$$

Next, we suppose the tensor valued function  $\hat{\mathcal{F}}$  to be invariant under superimposed rigid body motion, that is under the transformations of the type  $\mathbf{F} \rightarrow \mathbf{Q}\mathbf{F}$ ,  $\mathbf{H} \rightarrow \mathbf{Q}\mathbf{H}$ ,  $\mathbf{K} \rightarrow \mathbf{K}$ , and  $\mathbf{P} \rightarrow \mathbf{Q}\mathbf{P}$ , where  $\mathbf{Q} \in Orth^+$ . Further, if we assume  $\mathbf{Q} = \mathbf{H}^T \in Orth^+$ , then under SRBM,  $\mathbf{H} \rightarrow \mathbf{I}$ ,  $\dot{\mathbf{H}} \rightarrow \Omega \in Skw$ ,  $\mathbf{F} \rightarrow \mathbf{K}^{-1}$ ,  $\mathbf{K} \rightarrow \mathbf{K}$ , and  $\mathbf{P} \rightarrow \mathbf{H}^T\mathbf{P}$ . Since  $\Omega$  makes no contribution to the dissipation (cf. (4.57)), we introduce a constitutive assumption that  $\Omega = 0$ . Obtain

$$\begin{aligned} & \hat{\mathcal{F}}(\mathbf{K}^{-1}\dot{\mathbf{K}}, \mathbf{H}, \dot{\mathbf{H}}, J_K\mathbf{K}^T\mathbf{F}^T\mathbf{P}\mathbf{K}^{-T}, J_K\mathbf{K}^T(\mathbf{F}^T\mathbf{P})\mathbf{K}^{-T}) \\ &= \mathcal{K}(\mathbf{K}^{-1}\dot{\mathbf{K}}, J_K\mathbf{H}^T\mathbf{P}\mathbf{K}^{-T}, J_K\mathbf{K}^T(\mathbf{F}^T\mathbf{P})\mathbf{K}^{-T}) \\ &= \mathcal{K}(\mathbf{K}^{-1}\dot{\mathbf{K}}, \mathbf{S}, \dot{\mathbf{S}}), \end{aligned} \quad (4.63)$$

where  $\mathbf{S} = \mathbf{H}^T\mathbf{T}\mathbf{H}$  and  $\mathcal{K}$  is some tensor valued function. We also used the identity,  $\dot{\mathbf{S}} = J_K\mathbf{K}^T(\mathbf{F}^T\mathbf{P})\mathbf{K}^{-T} + (\mathbf{K}^{-1}\dot{\mathbf{K}})^T\mathbf{S} + \text{tr}(\mathbf{K}^{-1}\dot{\mathbf{K}})\mathbf{S} - \mathbf{S}(\mathbf{K}^{-1}\dot{\mathbf{K}})^T$ . The flow rule for an

elastically rigid perfectly plastic body therefore takes the form

$$\mathcal{K}(\mathbf{K}^{-1}\dot{\mathbf{K}}, \mathbf{S}, \dot{\mathbf{S}}) = \mathbf{0}. \quad (4.64)$$

For (isothermal) perfect plasticity, we cannot always solve (4.64) for  $\mathbf{K}^{-1}\dot{\mathbf{K}}$  explicitly as a function of  $\mathbf{S}$  and  $\dot{\mathbf{S}}$  (cf. (3.130)). To elaborate, consider the one dimensional example illustrated in Figure 1.1(i). During the rate independent plastic flow, the stress is constant (given by the yield limit), and therefore the stress rate vanishes. The plastic strain rate, however, need not be constant (it can be varied through the boundary). Therefore, we cannot express plastic strain rate as an explicit function of stress and stress rate. It can be shown that the plastic strain rate, in this case, is obtained only by solving the complete boundary value problem [82].

**Ilyushin's postulate** The assumption of an elastically rigid response implies that the internal work expended by the total strain vanishes for the processes which satisfy  $H(\mathbf{S}) < 0$ , where  $H(\mathbf{S}) = 0$  defines the yield manifold. Further, the assumption of a perfectly plastic response imply that the yield surface does not evolve in a loading process. Therefore, work is only performed by trajectories of the stress  $\mathbf{S}$ , which stay on the yield surface. It can then be deduced that the postulate Ilyushin [80] is equivalent to the dissipation hypothesis (4.57). Indeed, the postulate of Ilyushin states that for a closed cycle (in terms of  $\mathbf{F}$ ), which begins inside (or on) the yield surface, the net working by internal strain (at a fixed material point) is positive. That is for time  $t \in [t_1, t_2]$ , such that  $\mathbf{F}(t_1) = \mathbf{F}(t_2)$ , we require

$$\int_{t_1}^{t_2} \mathbf{P}(t) \cdot \dot{\mathbf{F}}(t) dt \geq 0. \quad (4.65)$$

If the process remains on the yield surface for a time  $[t_a, t_b] \subset [t_1, t_2]$ , then for an elastically rigid response, the above postulate reduces to,

$$\int_{t_a}^{t_b} \mathbf{P}(t) \cdot \dot{\mathbf{F}}(t) dt \geq 0. \quad (4.66)$$

This integral inequality can be localized on the manifold given by the yield condition, as the thermodynamic state remains on that manifold for any arbitrary time given by  $[t_a, t_b]$ . We also assume that the integrand is sufficiently smooth on the yield surface. On localizing we obtain

$$\mathbf{P}(t) \cdot \dot{\mathbf{F}}(t) \geq 0 \quad (4.67)$$

for the processes which are constrained to remain on the manifold of yield surface. Therefore for the case of elastically rigid perfect plasticity, Ilyushin's postulate implies the dissipation hypothesis (4.57). The converse is also true and can be proved on reversing the aforementioned steps.

The dissipation hypothesis, when expressed in terms of  $\mathbf{S}$ , reads as

$$\mathbf{S} \cdot \mathbf{K}^{-1} \dot{\mathbf{K}} < 0, \quad (4.68)$$

where  $\mathbf{S}$  remains on the yield manifold, defined by  $H(\mathbf{S}) = 0$  (and therefore  $\dot{\mathbf{K}} \neq \mathbf{0}$ ). We have seen that Ilyushin's condition does not imply the maximum dissipation postulate. However, Drucker's postulate remains valid [109], which does imply the inequality of maximum dissipation. Therefore, following the procedure discussed earlier, we can obtain an associated flow rule of the form

$$\mathbf{K}^{-1} \dot{\mathbf{K}} = \gamma H_{\mathbf{S}}, \quad (4.69)$$

where  $\gamma \geq 0$  is a scalar function. Moreover, since the skew part of  $\mathbf{K}^{-1} \dot{\mathbf{K}}$  makes no



contribution to the dissipation in (4.68), we can make the following constitutive assumption (cf. (3.134) and (4.23))

$$\mathbf{K}^{-1}\dot{\mathbf{K}} \in Sym. \quad (4.70)$$

*Remark 4.3.1.* (Levy–St. Venant relation) Assume a Mises type yield criteria (for isotropy), which is insensitive to pressure, such that

$$H_{\mathbf{S}} = \mathbf{S}^d, \quad (4.71)$$

where  $\mathbf{S}^d$  is the deviatoric part of  $\mathbf{S}$ . The flow rule (4.69) yields

$$Sym(\mathbf{K}^{-1}\dot{\mathbf{K}}) = \gamma \mathbf{S}^d. \quad (4.72)$$

Here  $\gamma$  is a scalar function such that it is invariant under the transformations which belong to the symmetry group of  $\kappa_i$  (here, that for isotropic materials). For  $\mathbf{H} \in Orth^+$ , we have,  $\dot{\mathbf{F}}\mathbf{F}^{-1} = \dot{\mathbf{H}}\mathbf{H}^T + \mathbf{H}\mathbf{K}^{-1}\dot{\mathbf{K}}\mathbf{H}^T$  and therefore  $\mathbf{D} \equiv Sym(\dot{\mathbf{F}}\mathbf{F}^{-1}) = \mathbf{H}Sym(\mathbf{K}^{-1}\dot{\mathbf{K}})\mathbf{H}^T$ . Also, the relation  $\mathbf{S} = \mathbf{H}^T\mathbf{T}\mathbf{H}$  implies that  $\text{tr } \mathbf{S} = \text{tr } \mathbf{T}$ . Therefore,  $\mathbf{S}^d = \mathbf{H}^T\mathbf{T}\mathbf{H} - \frac{1}{3}(\text{tr } \mathbf{T})\mathbf{1} = \mathbf{H}^T\mathbf{T}^d\mathbf{H}$ . The flow rule (4.72) can then be rewritten as

$$\mathbf{D} = \lambda \mathbf{T}^d, \quad (4.73)$$

which is the classical Levy–St. Venant relation for elastically rigid perfectly plastic solids (for isotropic materials) [82].

### 4.3.2 Example of a yield criterion and a flow rule

The yield condition is further subjected to the following restrictions due to material symmetry,

$$H(\mathbf{S}) = H(\mathbf{G}^T\mathbf{S}\mathbf{G}) \quad (4.74)$$

where  $\mathbf{G}$  is an element of the symmetry group of the intermediate configuration. The classical Mises condition, for isotropic material symmetry, is given by  $2J_2(\mathbf{T}^d) \equiv \mathbf{T}^d \cdot \mathbf{T}^d = 2k^2$ , where  $J_2(\mathbf{T}^d)$  denotes the second invariant of the Cauchy stress deviator and  $k$  is a constant for perfectly plastic behavior. The second invariant can be expanded in terms of the cartesian components of Cauchy stress tensor as

$$\begin{aligned} J_2(\mathbf{T}^d) &= \frac{1}{6} \left( (T_x - T_y)^2 + (T_x - T_z)^2 + (T_y - T_z)^2 \right) + (T_{xy}^2 + T_{xz}^2 + T_{yz}^2) \\ &= \frac{1}{6} \left( (T_x^d - T_y^d)^2 + (T_x^d - T_z^d)^2 + (T_y^d - T_z^d)^2 \right) + \left( (T_{xy}^d)^2 + (T_{xz}^d)^2 + (T_{yz}^d)^2 \right), \end{aligned}$$

where the second equality can be easily shown to follow from the identity,  $\mathbf{T}^d = \mathbf{T} - \frac{1}{3}(\text{tr } \mathbf{T})\mathbf{1}$ .

An extension of Mises criteria to materials demonstrating cubic symmetry can be obtained by following the example of Cazacu and Barlat [28], who treated the case of orthotropy. A generalized  $J_2$  (call it  $J_2^c$ ) is defined by writing down a second order homogeneous polynomial in stress, which is invariant with respect to the cubic symmetry group. A further restriction of its insensitivity to pressure is also imposed. We assume

$$J_2^c(\mathbf{T}^d) = \frac{m_1}{6} \left( (T_x^d - T_y^d)^2 + (T_x^d - T_z^d)^2 + (T_y^d - T_z^d)^2 \right) + m_2 \left( (T_{xy}^d)^2 + (T_{xz}^d)^2 + (T_{yz}^d)^2 \right), \quad (4.75)$$

where  $m_1$  and  $m_2$  are constants. Therefore, the modified Mises criteria for materials with cubic symmetry is given by

$$H(\mathbf{S}^d) = J_2^c - k^2 = 0. \quad (4.76)$$

The yield criteria (4.76) satisfies the symmetry relation (4.74) by construction (for a cubic symmetry group).

Next, we use the yield criterion (4.76) in the normality rule (4.69) to obtain a specific flow rule for materials with cubic symmetry. An indifference to pressure is also

assumed. Obtain

$$H_{\mathbf{S}^d} = \mathbf{T}_{\mathbf{S}^d}^d [(J_2^c)_{\mathbf{T}^d}] = \mathbf{H}^T (J_2^c)_{\mathbf{T}^d} \mathbf{H}, \quad (4.77)$$

where we have used the relation  $\mathbf{T}^d = \mathbf{H}\mathbf{S}^d\mathbf{H}^T$  to obtain the second equality. Further, the identity  $Sym(\mathbf{K}^{-1}\dot{\mathbf{K}}) = \mathbf{H}^T\mathbf{D}\mathbf{H}$  enables us to write the flow rule (4.69) as

$$\mathbf{D} = \lambda (J_2^c)_{\mathbf{T}^d}. \quad (4.78)$$

Use the expression for  $J_2^c$  from (4.75) to write the cartesian components of  $(J_2^c)_{\mathbf{T}^d}$

$$((J_2^c)_{\mathbf{T}^d})_{ij} = \frac{1}{2} \left( \frac{\partial J_2^c}{\partial T_{ij}^d} + \frac{\partial J_2^c}{\partial T_{ji}^d} \right) = \begin{pmatrix} m_1 T_x^d & m_2 T_{xy}^d & m_2 T_{xz}^d \\ m_2 T_{xy}^d & m_1 T_y^d & m_2 T_{yz}^d \\ m_2 T_{xz}^d & m_2 T_{yz}^d & m_1 T_z^d \end{pmatrix}. \quad (4.79)$$

Therefore, in terms of cartesian components of  $\mathbf{D}$  we have

$$\begin{pmatrix} D_x & D_{xy} & D_{xz} \\ D_{xy} & D_y & D_{yz} \\ D_{xz} & D_{yz} & D_z \end{pmatrix} = \lambda \begin{pmatrix} m_1 T_x^d & m_2 T_{xy}^d & m_2 T_{xz}^d \\ m_2 T_{xy}^d & m_1 T_y^d & m_2 T_{yz}^d \\ m_2 T_{xz}^d & m_2 T_{yz}^d & m_1 T_z^d \end{pmatrix}. \quad (4.80)$$

The above relation can be used in conjunction with the yield relation (4.76) to obtain  $\lambda$  in terms of  $\mathbf{D}$  and material constants.

### 4.3.3 Lüders bands

In this subsection we revisit the classical theory of Lüders Bands [165], but now extending it to materials with cubic symmetry. These bands consist of plastically deforming material, and are contained between two inclined planes bounded by rigid regions. We assume the material to be incompressible. The material velocity is assumed to be constant (with respect to time) in the plastic region and is assumed to vanish in the rigid region.

**Governing equations and jump conditions** For an incompressible material which displays cubic symmetry, we recall the flow rule and the yield condition from the previous subsection (equations (4.78) and (4.76), respectively). Therefore, with addition of the stress equilibrium (equation (2.146) with  $\mathbf{b} = \mathbf{0}$  and  $\dot{\mathbf{v}} = \mathbf{0}$ ), the following constitute the set of governing equations:

$$\operatorname{div} \mathbf{T} = \mathbf{0}, \quad (\text{Equilibrium})$$

$$\mathbf{D} = \lambda(J_2^c)_{\mathbf{T}^d}, \quad \text{and} \quad (\text{Flow rule})$$

$$J_2^c(\mathbf{T}^d) = k^2, \quad (\text{Modified Mises Yield Condition})$$

where the flow rule and the yield condition are valid only in the plastic part of the material. The jump conditions can be obtained at the interface between rigid and plastic medium. Let  $u$  denote the normal velocity of the interface. The normal is denoted by  $\mathbf{n}$  and we place a bar over the variables for rigid medium. The jump conditions are given by (cf. (2.133) and (2.148))

$$\rho(\mathbf{v} \cdot \mathbf{n} - u) = \bar{\rho}(\bar{\mathbf{v}} \cdot \mathbf{n} - u), \quad \text{and} \quad (4.81)$$

$$\llbracket \mathbf{T} \rrbracket \mathbf{n} = \rho(\mathbf{v} \cdot \mathbf{n} - u) \llbracket \mathbf{v} \rrbracket, \quad (4.82)$$

where  $\rho$  denotes the density and  $\mathbf{v}$ , the material velocity. Since the material in the rigid part is at rest, we have  $\bar{\mathbf{v}} = \mathbf{0}$ . We can then substitute the first jump condition into the second to obtain

$$\llbracket \mathbf{T} \rrbracket \mathbf{n} = -\bar{\rho} u \mathbf{v}. \quad (4.83)$$

**An ideal flat bar** As an illustrative example, we consider an ideal flat rectangular bar, whose flat sides are formed by two infinite parallel planes. We can define a convenient carte-

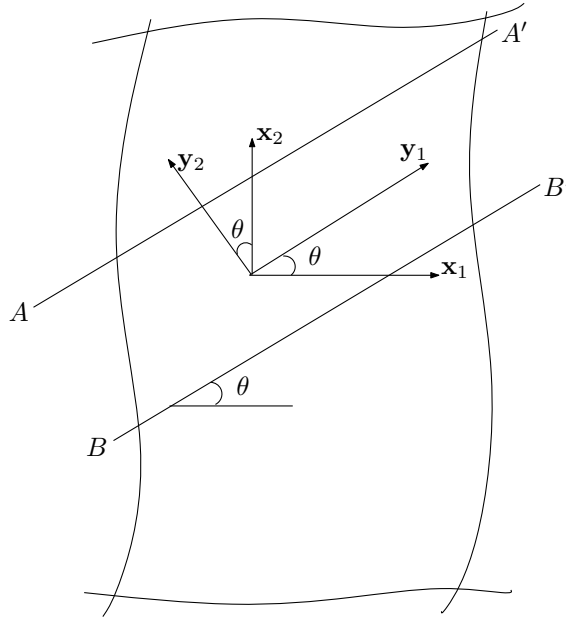


Figure 4.2: Portion of an ideal flat bar. (After Thomas [165]).

sian coordinate system, given by orthogonal triplets  $(\mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_3)$  such that  $\mathbf{y}_1$  lies parallel to the band,  $\mathbf{y}_2$  in the direction of normal to the interface between and plastic and rigid media (cf. Figure 4.2, where the plastic medium is restricted between planes  $AA'$  and  $BB'$ ), and therefore  $\mathbf{y}_3$  points out of the plane of paper, through the free surface of the bar. We have the following relation between two coordinate systems shown in Figure 4.2:

$$\mathbf{x}_1 = \mathbf{y}_1 \cos \theta - \mathbf{y}_2 \sin \theta,$$

$$\mathbf{x}_2 = \mathbf{y}_1 \sin \theta + \mathbf{y}_2 \cos \theta, \text{ and}$$

$$\mathbf{x}_3 = \mathbf{y}_3.$$

Let the bar be subjected to uniaxial stress of magnitude  $Y$  in the direction of  $\mathbf{x}_2$ .

Therefore, the state of stress  $\Sigma$  in the rigid part of the bar is given by

$$\Sigma = Y \mathbf{x}_2 \otimes \mathbf{x}_2 = Y \sin^2 \theta \mathbf{y}_1 \otimes \mathbf{y}_1 + Y \sin \theta \cos \theta (\mathbf{y}_1 \otimes \mathbf{y}_2 + \mathbf{y}_2 \otimes \mathbf{y}_1) + Y \cos^2 \theta \mathbf{y}_2 \otimes \mathbf{y}_2. \quad (4.84)$$

Our aim is to find the inclination angle  $\theta$ , which the plastic band makes with the horizontal plane. We consider a simple solution of the velocity field in the plastic region

$$\mathbf{v} = ay_2\mathbf{y}_1 + by_2\mathbf{y}_2 - by_3\mathbf{y}_3, \quad (4.85)$$

where  $a$  and  $b$  are constants. Note, that the condition of incompressibility is satisfied immediately with this velocity field ( $\text{div } \mathbf{v} = 0$ ). The velocity field in (4.85) should also satisfy jump conditions (4.81) and (4.83) and also the condition which requires vanishing of the traction on the free surface (which is normal to  $\mathbf{y}_3$ ). From the above velocity field we obtain

$$\mathbf{D} = \text{Sym}(\text{grad } \mathbf{v}) = by_2 \otimes \mathbf{y}_2 + \frac{a}{2}(\mathbf{y}_1 \otimes \mathbf{y}_2 + \mathbf{y}_2 \otimes \mathbf{y}_1) - by_3 \otimes \mathbf{y}_3. \quad (4.86)$$

Using the flow rule in the component form from (4.80), we can obtain the following stress field in the plastic region:

$$\mathbf{T}^d = \frac{b}{\lambda m_1} \mathbf{y}_2 \otimes \mathbf{y}_2 + \frac{a}{2\lambda m_2} (\mathbf{y}_1 \otimes \mathbf{y}_2 + \mathbf{y}_2 \otimes \mathbf{y}_1) - \frac{b}{\lambda m_1} \mathbf{y}_3 \otimes \mathbf{y}_3 \quad (4.87)$$

and therefore

$$\mathbf{T} = -p\mathbf{y}_1 \otimes \mathbf{y}_1 \left( \frac{b}{\lambda m_1} - p \right) \mathbf{y}_2 \otimes \mathbf{y}_2 + \frac{a}{2\lambda m_2} (\mathbf{y}_1 \otimes \mathbf{y}_2 + \mathbf{y}_2 \otimes \mathbf{y}_1) - \left( \frac{b}{\lambda m_1} + p \right) \mathbf{y}_3 \otimes \mathbf{y}_3, \quad (4.88)$$

where  $p = -\frac{1}{3} \text{tr } \mathbf{T}$ . Substituting  $\mathbf{T}$  in the equilibrium condition furnishes  $\text{grad } p = \mathbf{0}$ . Therefore  $p$  is constant within the plastic region. The traction on the free surface is given by  $\mathbf{T}\mathbf{y}_3$ . Vanishing of this traction implies that  $p = -\frac{b}{\lambda m_1}$  over the outer boundaries of the band, and also inside the whole plastic band (since  $p$  is constant in the plastic region). Moreover, the jump condition (4.81) provides us with the relation (with  $\mathbf{n} = \mathbf{y}_2$ )

$$\rho b \hat{y}_2 = u(\rho - \bar{\rho}), \quad (4.89)$$

where  $\hat{y}_2$  is the half-width of the plastic band. The jump condition (4.83), on the other hand, gives us

$$\llbracket T_{i2} \rrbracket = T_{i2} - \Sigma_{i2} = -\bar{\rho}uv_i \quad (4.90)$$

from which we obtain the following two conditions,

$$\frac{a}{2\lambda m_2} - Y \sin \theta \cos \theta = -\bar{\rho}ua\hat{y}_2. \quad (4.91)$$

$$\frac{2b}{\lambda m_1} - Y \cos^2 \theta = -\bar{\rho}ub\hat{y}_2. \quad (4.92)$$

Divide above relations with respect to each other to obtain

$$\tan \theta = \frac{m_1 a (1 + 2\lambda m_2 \bar{\rho} u \hat{y}_2)}{2m_2 b (2 + \lambda m_1 \bar{\rho} u \hat{y}_2)}. \quad (4.93)$$

We eliminate  $\theta$  from these equations by using the identity  $1 + \tan^2 \theta = \sec^2 \theta$  and the relations (4.92) and (4.93) to get,

$$\frac{4m_2^2 b^2 (2 + \lambda m_1 \bar{\rho} u \hat{y}_2)^2 + m_1^2 a^2 (1 + 2\lambda m_2 \bar{\rho} u \hat{y}_2)^2}{4m_1 m_2^2 b (2 + \lambda m_1 \bar{\rho} u \hat{y}_2)} = \lambda Y. \quad (4.94)$$

Substitute the components of the stress state given in equation (4.87) into relation (4.75) and then use the result in the yield equation (4.76) to obtain

$$\frac{b^2}{m_1} + \frac{a^2}{4m_2} = \lambda^2 k^2 = \frac{m_1 \lambda^2 Y^2}{3}, \quad (4.95)$$

which can be rewritten as (denoting  $c = \frac{a}{b}$ ),

$$\lambda^2 = \frac{3u^2(\rho - \bar{\rho})^2}{m_1 \rho^2 \hat{y}_2^2 Y^2} \left( \frac{1}{m_1} + \frac{c^2}{4m_2} \right), \quad (4.96)$$

where we have used equation (4.89) to replace  $b$ . A nonlinear equation in  $c$  is then obtained by substituting  $\lambda$  from (4.96) into (4.94). After solving for  $c$ , we can obtain  $\lambda$  from (4.96) and subsequently  $\theta$  from (4.93).

## Chapter 5

# Surface Dislocations and Plastic Waves

This chapter is divided into two parts. The first part deals with the general theory of surface dislocation density and the second part is concerned with the theory of adiabatic plastic waves. A wave is understood to be a moving singular surface, across which fields and their derivatives might suffer jump discontinuities. We discuss waves across which thermodynamic state variables are discontinuous (shock waves) and waves across which state variables are continuous but their first derivatives are discontinuous (acceleration waves). In particular, we emphasize the role of dislocation distribution in the neighborhood of the wave. In shock waves, there exists a possibility of the formation of walls of dislocations which propagate with the shock. On the other hand in acceleration waves, such walls cannot exist, but an important role is played by the bulk dislocation content which lies close to the wave.



In Subsection 5.1.1 of Section 5.1, we introduce the concept of surface dislocation density arising from a discontinuous plastic distortion or a discontinuous elastic distortion. For a nonzero surface dislocation density, the jumps in  $\mathbf{K}$  and  $\mathbf{H}$  are not rank one, unlike the jump in  $\mathbf{F}$  (cf. (2.65)). We also obtain compatibility conditions to be satisfied at a surface dislocation node, which is the line at which several dislocated surfaces intersect. In Subsection 5.1.2, a measure of surface dislocation density, which is invariant with respect to compatible changes in the reference configuration, is obtained. Finally in Subsection 5.1.3, the jump in bulk dislocation density is related to the surface dislocation density. For a moving surface, the jump is given completely in terms of the jump in plastic distortion rate and the surface dislocation density. In particular, we obtain in (5.68) a statement of the conservation of dislocation density at the surface, according to which the normal component of the jump in bulk dislocation density is equal to the surface divergence of the surface dislocation density.

Section 5.2 is concerned with adiabatic shock waves in elastic-plastic solids. Shock waves are defined as moving singular surfaces across which thermodynamic state variables are discontinuous. After stating the relevant compatibility conditions and Hugoniot relations, we discuss, in Subsection 5.2.1, some general results for elastic shock waves. In particular we show that the jump in entropy is of the third order in the jump in deformation gradient, and the change in entropy is of the same sign as of the change in shock speed. The necessity of Legendre–Hadamard condition and the genuine nonlinearity is emphasized. In Subsection 5.2.2 on plastic shock waves, we investigate on how the results of elastic shocks modify due to the presence of plastic flow at the shock surface. We find that

the jump in entropy, for fixed plastic flow, is of the first order in the jump in deformation gradient. Furthermore, we show that Legendre–Hadamard condition is no more necessary for the existence of shocks. In the last subsection, we consider the shock as a dislocation wall, i.e. a surface with dislocation distribution. Using results from Section 5.1 we obtain simple equations, which for given material parameters can be used to determine dislocation density distribution at the shock as well as the shock speed. Results are obtained for both isotropic and cubic material symmetry.

The last section in this chapter deals with adiabatic acceleration waves in elastic–plastic solids. Acceleration waves are defined as moving singular surfaces, across which thermodynamic state variables are continuous, but their derivatives are discontinuous. The form of governing equations for acceleration waves make them much more analytically tractable than shock waves. In many simple cases, wave speeds can be determined even for a three dimensional case. After developing the general theory of elastic–plastic acceleration waves, we consider specific models of elastic and plastic acceleration waves. Some classical results on the form of elastic acoustic tensor for isotropic and cubic material symmetry are derived. In the last subsection on plastic acceleration waves, rate–independent behavior is assumed and the resulting theory is formulated with and without hardening.

## 5.1 Dislocation distribution at the interface

Consider a singular surface  $S_t \subset \kappa_r$ , with normal  $\mathbf{N}$  and normal velocity  $U$  (cf. Subsection 2.1.4). For smooth deformations, we obtained, in equation (2.65), a compatibility condition for  $\mathbf{F}$  as  $[[\mathbf{F}]] = \mathbf{a} \otimes \mathbf{N}$ , where  $\mathbf{a} \in \mathcal{V}$  is arbitrary. Below, we obtain compatibility

conditions for plastic and elastic deformation maps and interpret them in terms of *surface dislocations*. The concept of surface dislocation density was introduced by Bilby [12, 25, 13] as a smeared out defect distribution at an interface separating differently oriented/strained domains. Bilby's work attempted to generalize the earlier models of dislocation content at grain boundaries as proposed by Burgers [26], Bragg [16], and Frank [54]. A physically meaningful interpretation as a two dimensional array of dislocations is possible only for low values of surface dislocation density, since individual dislocations can not be placed arbitrarily closed to each other ([35], sec. 38). Examples include simple tilt boundaries [26], low angle grain boundaries [149], and shock waves [158].

In Subsection 5.1.3, higher order compatibility conditions are used to investigate the interplay between bulk and surface dislocation densities. For a moving interface, the jump in bulk dislocation density is related to the jump in plastic distortion rate and derivatives of surface dislocation density. Such a relation is useful in situations where a moving interface modifies the defect structure in the bulk as it traverses through it.

### 5.1.1 Surface dislocation density

Recall, from Chapter 3, the definition of Burgers vector

$$B(C, t) = \oint_C \mathbf{K}^{-1} d\mathbf{X}, \quad (5.1)$$

where  $C$  is a close material curve which intersects  $S_t$  in finite number of points and  $\mathbf{K}^{-1}$  is piecewise smooth. This restriction on  $C$  is to ensure that the integral in (5.1) is well defined. The plastic deformation  $\mathbf{K}^{-1}$  is singular on  $S_t$ , and therefore the integral in (5.1) will have singularities only over a set of measure zero (a finite collection of points on a line constitute

such a set). Let  $A_C$  be the area of the surface enclosed by  $C$  and let  $\Gamma = A_C \cap S_t$  be the curve which lies at the intersection of  $A_C$  and  $S_t$ . Use the Stokes' theorem for piecewise continuous tensor fields (2.103) to obtain

$$\oint_C \mathbf{K}^{-1} d\mathbf{X} = \int_{A_C} (\text{Curl } \mathbf{K}^{-1})^T \mathbf{N}_C dA - \int_{\Gamma} \llbracket \mathbf{K}^{-1} \rrbracket d\mathbf{X}, \quad (5.2)$$

where  $\mathbf{N}_C$  is the unit normal field associated with  $A_C$ . The equation for Burgers vector thus becomes

$$B(C, t) = \int_{A_C} (\text{Curl } \mathbf{K}^{-1})^T \mathbf{N}_C dA - \int_{\Gamma} \llbracket \mathbf{K}^{-1} \rrbracket d\mathbf{X}. \quad (5.3)$$

Let  $\{\mathbf{t}_1, \mathbf{t}_2\} \in T_{S_t(X)}$ , where  $T_{S_t(X)}$  denotes the tangent space to  $S_t$  at  $\mathbf{X}$ , be such that  $\{\mathbf{t}_1, \mathbf{t}_2, \mathbf{N}\}$  is a positively-oriented orthonormal basis. Furthermore, let  $\mathbf{t}_2$  be oriented along the curve  $\Gamma$ , so that  $d\mathbf{X} = \mathbf{t}_2 du = (\mathbf{N} \times \mathbf{t}_1) du$  in the final integral in (5.3), where  $u$  measures arc-length on  $\Gamma$ . We define a tensor field  $\beta_r$  on  $S_t$ , the (referential) *surface dislocation density*, such that

$$\llbracket \mathbf{K}^{-1} \rrbracket (\mathbf{t}_1 \times \mathbf{N}) = \beta_r^T \mathbf{t}_1. \quad (5.4)$$

The net Burgers vector associated with  $C$  is then given by

$$B(C, t) = \int_{A_C} \alpha_r^T \mathbf{N}_C dA + \int_{\Gamma} \beta_r^T \mathbf{t}_1 du. \quad (5.5)$$

Writing  $\llbracket \mathbf{K}^{-1} \rrbracket = \llbracket \mathbf{K}^{-1} \rrbracket \mathbf{1}$  with  $\mathbf{1} = \mathbf{N} \otimes \mathbf{N} + \mathbf{t}_a \otimes \mathbf{t}_a$  ( $a = 1, 2$ ), (5.4) leads to

$$\llbracket \mathbf{K}^{-1} \rrbracket = \mathbf{k} \otimes \mathbf{N} - \beta_r^T \varepsilon_{(\mathbf{N})}, \quad (5.6)$$

where  $\mathbf{k}$  is an arbitrary 3-vector and

$$\varepsilon_{(\mathbf{N})} = \mathbf{t}_1 \otimes \mathbf{t}_2 - \mathbf{t}_2 \otimes \mathbf{t}_1 \quad (5.7)$$

is the two-dimensional permutation tensor density on  $T_{S_t(X)}$ . This satisfies  $\boldsymbol{\varepsilon}_{(\mathbf{N})} = \mathbf{R}\boldsymbol{\varepsilon}_{(\mathbf{N})}\mathbf{R}^T$  for all two-dimensional orthogonal transformations  $\mathbf{R}$  that preserve the orientation of  $T_{S_t(X)}$ . Therefore any pair of vectors in  $T_{S_t(X)}$  which with  $\mathbf{N}$  form a positive orthonormal basis may be used in the definition of  $\boldsymbol{\varepsilon}_{(\mathbf{N})}$ .

Use  $\boldsymbol{\varepsilon}_{(\mathbf{N})}^2 = -\mathbb{P}$  in (5.6), where  $\mathbb{P} = \mathbf{1} - \mathbf{N} \otimes \mathbf{N}$  is the identity for  $T_{S_t(X)}$ , to obtain

$$\boldsymbol{\beta}_r^T \mathbb{P} = \llbracket \mathbf{K}^{-1} \rrbracket \boldsymbol{\varepsilon}_{(\mathbf{N})}. \quad (5.8)$$

This determines the action of  $\boldsymbol{\beta}_r^T$  on  $T_{S_t(X)}$ . The action of  $\boldsymbol{\beta}_r^T$  on  $\mathbf{N}$  is indeterminate and may be set to zero without loss of generality. Thus we can consider  $\boldsymbol{\beta}_r^T$  to be a superficial tensor (i.e.  $\boldsymbol{\beta}_r^T \mathbb{P} = \boldsymbol{\beta}_r^T$ ) and write

$$\boldsymbol{\beta}_r^T = \llbracket \mathbf{K}^{-1} \rrbracket \boldsymbol{\varepsilon}_{(\mathbf{N})}. \quad (5.9)$$

The formula (5.9) is equivalent to a result stated by Bilby ([12], equation 10) and used extensively in the subsequent literature on crystal interfaces and grain boundaries [135, 10]. Bilby's result is not consistent with his definition of surface dislocation density as stated in the text of [12]. He defines the latter to be the finite limit obtained by invoking Stokes' theorem, collapsing  $A_C$  onto  $\Gamma$ , and requiring the dislocation density  $\boldsymbol{\alpha}_r$  to become unbounded. However, the indicated limit vanishes under conditions in which Stokes' theorem is valid.

The interface  $S_t$  is *coherent* at  $\mathbf{X} \in S_t$  if the Burgers vector, as defined in (5.5), has no contributions from the line integral, for all closed curves  $C$  such that  $\mathbf{X} \in \Gamma$ , where  $\Gamma = S_t \cap A_C$ . Assume  $\boldsymbol{\beta}_r^T$  to be superficial. It then follows from (5.5), that  $S_t$  is *coherent* at  $\mathbf{X} \in S_t$  if and only if the surface dislocation density  $\boldsymbol{\beta}_r^T$  at  $\mathbf{X}$  vanishes. For a zero surface dislocation density, (5.6) yields Hadamard's formula  $\llbracket \mathbf{K}^{-1} \rrbracket = \mathbf{k} \otimes \mathbf{N}$ .

If  $\mathbf{K}^{-1}$  is the gradient of a piecewise continuously differentiable deformation  $\chi^p$ , i.e.  $\mathbf{K}^{-1} = \nabla \chi^p$ , then following the analysis which led to (2.69), we obtain

$$\llbracket \mathbf{K}^{-1} \rrbracket = \mathbf{k} \otimes \mathbf{N} + \nabla^S \llbracket \chi^p \rrbracket. \quad (5.10)$$

The surface dislocation density, given by (5.8), then has the form

$$\beta_r^T \mathbb{P} = \nabla^S \llbracket \chi^p \rrbracket \varepsilon_{(\mathbf{N})} = \nabla \llbracket \chi^p \rrbracket \varepsilon_{(\mathbf{N})}, \quad (5.11)$$

where the second equality is obtained using definition (2.54) and the identity  $\mathbb{P} \varepsilon_{(\mathbf{N})} = \varepsilon_{(\mathbf{N})}$ . This situation occurs when the bulk dislocation density  $\boldsymbol{\alpha}^r = \text{Curl } \mathbf{K}^{-1}$  vanishes, on either side of the interface, and the dislocation distribution is restricted to the singular surface  $S_t$ . Equation (5.6) extend Hadamard's result to general non-coherent (i.e., dislocated) interfaces and equation (5.10) extend it to the non-coherent interface with vanishing bulk dislocation density in the neighborhood.

*Remark 5.1.1.* In a situation where  $\beta_r^T$  is given by (5.11), a necessary and sufficient condition for it to vanish on  $S_t$  is  $\llbracket \chi^p \rrbracket = \mathbf{c}$ , a constant (on  $S_t$ ). The sufficiency of this condition is obvious. For necessity, put  $\beta_r^T = \mathbf{0}$  in (5.11) to get

$$\nabla^S \llbracket \chi^p \rrbracket \varepsilon_{(\mathbf{N})} = \mathbf{0}. \quad (5.12)$$

Multiply both sides by  $\varepsilon_{(\mathbf{N})}$  and use  $\varepsilon_{(\mathbf{N})}^2 = -\mathbb{P}$  to obtain  $\nabla^S \llbracket \chi^p \rrbracket \mathbb{P} = \mathbf{0}$ , which on noting the definition of the surface gradient (cf. (2.54)) and the identity  $\mathbb{P}^2 = \mathbb{P}$ , reduces to  $\nabla^S \llbracket \chi^p \rrbracket = \mathbf{0}$ , thereby implying that  $\llbracket \chi^p \rrbracket$  is constant at the surface.

Proceeding from (3.20) and (3.22)<sub>2</sub> instead, we derive

$$\llbracket \mathbf{H}^{-1} \rrbracket = \mathbf{h} \otimes \mathbf{n} - \beta_t^T \varepsilon_{(\mathbf{n})} \quad \text{and} \quad \beta_t^T \mathbb{P}_{(\mathbf{n})} = \llbracket \mathbf{H}^{-1} \rrbracket \varepsilon_{(\mathbf{n})}, \quad (5.13)$$

where  $\mathbf{h}$  is an arbitrary 3-vector,  $\mathbf{n}$  is the orientation of a surface  $s_t \subset \kappa_t$  of discontinuity of  $\mathbf{H}^{-1}(\mathbf{x}, t)$ ,  $\mathbb{P}_{(\mathbf{n})} = \mathbf{1} - \mathbf{n} \otimes \mathbf{n}$  is the (spatial) projection tensor, and  $\beta_t$  is the spatial surface dislocation density. The Burgers vector using spatial description is given by

$$\begin{aligned} \mathbf{b}(c, t) &= \int_c \mathbf{H}^{-1} d\mathbf{x} = \int_{A_c} (\text{curl } \mathbf{H}^{-1})^T \mathbf{n}_c da - \int_\gamma \llbracket \mathbf{H}^{-1} \rrbracket d\mathbf{x} \\ &= \int_{A_c} (\boldsymbol{\alpha}_t)^T \mathbf{n}_c da + \int_\gamma \beta_t^T \hat{\mathbf{t}}_1 d\hat{u}, \end{aligned} \quad (5.14)$$

where  $c$  is a (closed) spatial curve enclosing area  $A_c$  (with unit normal  $\mathbf{n}_c$ ) and  $\gamma = A_c \cap s_t$ . The curve  $\gamma$  is parameterized with arc-length  $\hat{u}$  and has an associated tangent vector, say  $\hat{\mathbf{t}}_2$ . The triad  $\{\hat{\mathbf{t}}_1, \hat{\mathbf{t}}_2, \mathbf{n}\}$  forms a positively oriented orthonormal basis on  $s_t$ , where  $\mathbf{n}$  is the unit normal associated with  $s_t$ .

If  $\mathbf{H}^{-1}$  is the gradient of a piecewise continuously differentiable deformation  $\boldsymbol{\chi}^e$ , i.e.  $\mathbf{H}^{-1} = \nabla \boldsymbol{\chi}^e$ , then equations (5.13) reduce to (cf. (5.10) and (5.11))

$$\llbracket \mathbf{H}^{-1} \rrbracket = \mathbf{h} \otimes \mathbf{n} + \nabla^s \llbracket \boldsymbol{\chi}^e \rrbracket \quad \text{and} \quad \beta_t^T \mathbb{P}_{(\mathbf{n})} = \nabla^s \llbracket \boldsymbol{\chi}^e \rrbracket \boldsymbol{\varepsilon}_{(\mathbf{n})}, \quad (5.15)$$

where  $\nabla^s$  is the surface gradient with respect to the spatial surface. This case has been previously discussed in [97, 105, 29], but equations (5.13) now extend their analysis to the case when dislocations are present even in the bulk surrounding the interface. Such an extension has been discussed earlier by Cermelli & Sellers [31] in the context of crystal lattice vectors.

Equation (5.13)<sub>1</sub> reduces in the coherent case (i.e. when  $\beta_t^T = \mathbf{0}$ ) to Hadamard's rank-one form  $\llbracket \mathbf{H}^{-1} \rrbracket = \mathbf{h} \otimes \mathbf{n}$ . Evidently the generalization to non-coherent interfaces yields a full-rank expression which relaxes the constraint on the limits  $(\mathbf{H}^{-1})^\pm$  associated with a coherent interface. Accordingly, surface dislocation is an additional interfacial degree of

freedom which is available to minimize the elastic energy in the adjoining material. In general, this implies that non-coherent interfaces are energetically optimal, which presumably accounts for the stress relaxation typically attributed to the mechanism of surface dislocation. For example, our constitutive hypotheses imply that adjoining crystal grains are in their minimum-energy states if  $\mathbf{H}^T \mathbf{H} = \mathbf{1}$  therein. By the polar decomposition theorem,  $\mathbf{H}^{-1}$  then reduces to a rotation in each grain, and (5.13)<sub>2</sub> furnishes the required surface dislocation density in terms of the rotation discontinuity (cf. [54]). The so-called *tilt* and *twist* boundaries furnish an illustrative example ([93], sec. 3.9).

The referential and spatial surface dislocation densities are not independent. For, if  $s_t$  is the image of  $S_t$  under the overall deformation, i.e. if  $s_t = \chi(S_t, t)$ , then the existence of a continuous inverse deformation  $\chi^{-1}(\mathbf{x}, t)$  mapping  $\kappa_t$  to  $\kappa_r$  implies that any jump in  $\mathbf{F}^{-1}$  has Hadamard's form  $[[\mathbf{F}^{-1}]] = \mathbf{a} \otimes \mathbf{n}$ . Using this in the inverse of (3.18) together with

$$[[\mathbf{H}^{-1}]] = \langle \mathbf{K}^{-1} \rangle [[\mathbf{F}^{-1}]] + [[\mathbf{K}^{-1}]] \langle \mathbf{F}^{-1} \rangle, \quad (5.16)$$

we derive

$$\mathbf{h} \otimes \mathbf{n} - \beta_t^T \boldsymbol{\varepsilon}_{(\mathbf{n})} = \langle \mathbf{K}^{-1} \rangle \mathbf{a} \otimes \mathbf{n} + \mathbf{k} \otimes \langle \mathbf{F}^{-T} \rangle \mathbf{N} - \beta_r^T \boldsymbol{\varepsilon}_{(\mathbf{N})} \langle \mathbf{F}^{-1} \rangle. \quad (5.17)$$

Nanson's formula ensures that  $\langle \mathbf{F}^{-T} \rangle \mathbf{N}$  is parallel to  $\mathbf{n}$ . Multiplication on the right by  $\boldsymbol{\varepsilon}_{(\mathbf{n})}$  thus furnishes  $\beta_t^T$  in terms of  $\beta_r^T$ :

$$\beta_t^T \mathbb{P}_{(\mathbf{n})} = -\beta_r^T \boldsymbol{\varepsilon}_{(\mathbf{N})} \langle \mathbf{F}^{-1} \rangle \boldsymbol{\varepsilon}_{(\mathbf{n})}, \quad (5.18)$$

and the normal component of (5.17) yields a relationship among the vectors  $\mathbf{a}$ ,  $\mathbf{k}$  and  $\mathbf{h}$ :

$$\mathbf{h} = \langle \mathbf{K}^{-1} \rangle \mathbf{a} + (\mathbf{n} \cdot \langle \mathbf{F}^{-T} \rangle \mathbf{N}) \mathbf{k} - \beta_r^T \boldsymbol{\varepsilon}_{(\mathbf{N})} \langle \mathbf{F}^{-1} \rangle \mathbf{n}. \quad (5.19)$$



*Remark 5.1.2.* (Surface dislocation nodes) A *surface dislocation node*, as introduced by Bilby [12], is the line of intersection of surfaces with dislocation distribution. The analysis in [12] is restricted to plane surfaces and infinitesimal strains. We extend it for curved surfaces and finite strains. Consider  $N$  surfaces intersecting at a line  $L \subset \kappa_r$ . Each surface has an associated normal and a distribution of surface dislocation density. The following compatibility relation holds in a neighborhood infinitesimal close to  $L$

$$\sum_{i=1}^N \llbracket \mathbf{K}^{-1(i)} \rrbracket = \mathbf{0}, \quad (5.20)$$

where the index  $i$  in the superscript represents the  $i$ 'th surface. This relation follows from the observation that, on passing around the line  $L$  (in a small neighborhood), one reaches the initial material point. Use (5.6) to obtain

$$\sum_{i=1}^N (\mathbf{k}^{(i)} \otimes \mathbf{N}^{(i)} - \beta_r^{T(i)} \boldsymbol{\varepsilon}_{(\mathbf{N}^{(i)})}) = \mathbf{0}. \quad (5.21)$$

Let  $\mathbf{t}$  be the unit tangent vector field associated with line  $L$ . We can therefore choose a vector  $\mathbf{t}^{(i)} \in T_{S_t^{(i)}}$  at  $\mathbf{X} \in L$  such that  $\{\mathbf{t}, \mathbf{t}^{(i)}, \mathbf{N}^{(i)}\}$  forms a positively oriented orthonormal basis at  $\mathbf{X} \in L$  for each intersecting surface. We also have (cf. (5.7))

$$\boldsymbol{\varepsilon}_{(\mathbf{N}^{(i)})} = \mathbf{t} \otimes \mathbf{t}^{(i)} - \mathbf{t}^{(i)} \otimes \mathbf{t}. \quad (5.22)$$

On substituting this in (5.21), it follows immediately that

$$\mathbf{0} = \sum_{i=1}^N \llbracket \mathbf{K}^{-1(i)} \rrbracket \mathbf{t} = \sum_{i=1}^N \beta_r^{T(i)} \mathbf{t}^{(i)} \quad (5.23)$$

at  $\mathbf{X} \in L$ . The outer equality in (5.23) provides us with a compatibility condition relating the surface dislocation density tensors of various intersecting surfaces. This can be compared to the equation of conservation of Burgers vectors. Equivalently, in terms of the spatial

surface dislocation density, we can obtain  $\sum_{i=1}^N \beta_t^{T(i)} \hat{\mathbf{t}}^{(i)} = \mathbf{0}$ , where  $\hat{\mathbf{t}}^{(i)} \in T_{S_t^{(i)}}$ . Surface dislocation nodes have been observed by Li et al. [106] during indentation of zinc crystals and by Basinski and Christian [9] in their study of martensitic transformations.

### 5.1.2 True surface dislocation density

In equation (3.23), a measure of the bulk dislocation in the *body*, the true dislocation density, was defined, and its invariance under compatible changes in the reference and the current configurations was demonstrated. We will now obtain an analogous measure for surface dislocation density. Consider two reference configurations,  $\kappa_{r_1}$  and  $\kappa_{r_2}$  such that there exists a map  $\boldsymbol{\lambda}$  such that  $\mathbf{X}_2 = \boldsymbol{\lambda}(\mathbf{X}_1)$ , where  $\mathbf{X}_1 \in \kappa_{r_1}$  and  $\mathbf{X}_2 \in \kappa_{r_2}$ , with invertible gradient  $\mathbf{A} = \nabla_1 \boldsymbol{\lambda}$  (such that  $\mathbf{K}_2 = \mathbf{A}\mathbf{K}_1$ ). For  $\mathbf{A}$  to be a compatible deformation from  $\kappa_{r_1}$  and  $\kappa_{r_2}$ , the Hadamard's rank one compatibility  $[[\mathbf{A}]] = \mathbf{d} \otimes \mathbf{N}$ , where  $\mathbf{d} \in \mathcal{V}$  is arbitrary, persists at the singular interface. Such a compatible transformation leaves the Burgers vector invariant and consequently it follows from (5.3) that

$$\int_{A_{C_1}} (\text{Curl}_1 \mathbf{K}_1^{-1})^T \mathbf{N}_{C_1} dA_1 - \int_{\Gamma_1} [[\mathbf{K}_1^{-1}]] d\mathbf{X}_1 = \int_{A_{C_2}} (\text{Curl}_2 \mathbf{K}_2^{-1})^T \mathbf{N}_{C_2} dA_2 - \int_{\Gamma_2} [[\mathbf{K}_2^{-1}]] d\mathbf{X}_2, \quad (5.24)$$

where  $A_{C_2} = \boldsymbol{\lambda}(A_{C_1})$  and  $\Gamma_2 = \boldsymbol{\lambda}(\Gamma_1)$ . Relations (3.25) and (3.26) ensure the equality of the area integrals in (5.24) and thereby reducing it to

$$\int_{\Gamma_1} [[\mathbf{K}_1^{-1}]] d\mathbf{X}_1 = \int_{\Gamma_2} [[\mathbf{K}_2^{-1}]] d\mathbf{X}_2. \quad (5.25)$$

Let  $\mathbf{t}_a$  and  $u_a$  be the unit tangent vector and the arc-length associated with  $\Gamma_a$ , respectively ( $a = 1, 2$ ). Then

$$\mathbf{t}_2 du_2 = d\mathbf{X}_2 = \mathbf{A}^\pm d\mathbf{X}_1 = \mathbf{A}^\pm \mathbf{t}_1 du_1, \quad (5.26)$$

where the superscript  $\pm$  implies that both  $+$  or  $-$  limits can be used in the formula (this follows from the compatibility of  $\mathbf{A}$ , i.e.  $\mathbf{A}^+\mathbf{t}_1 = \mathbf{A}^-\mathbf{t}_1$ ). Substituting  $d\mathbf{X}_2$  from (5.26) into (5.25) and using the arbitrariness of  $\Gamma_1$  we obtain

$$\llbracket \mathbf{K}_2^{-1} \rrbracket \mathbf{A}^\pm \mathbf{t}_1 = \llbracket \mathbf{K}_1^{-1} \rrbracket \mathbf{t}_1 \quad (5.27)$$

for  $\mathbf{t}_1 \in T_{S_{t_1}}$ . This relation is satisfied if the jump assumes the following form

$$\llbracket \mathbf{K}_2^{-1} \rrbracket \mathbf{A}^\pm - \llbracket \mathbf{K}_1^{-1} \rrbracket = \mathbf{c} \otimes \mathbf{N}_1, \quad (5.28)$$

where  $\mathbf{c} \in \mathcal{V}$  is arbitrary. Multiply both sides by  $\boldsymbol{\varepsilon}_{(\mathbf{N}_1)}$ . As a result, obtain

$$\llbracket \mathbf{K}_2^{-1} \rrbracket \mathbf{A}^\pm \boldsymbol{\varepsilon}_{(\mathbf{N}_1)} = \boldsymbol{\beta}_{r_1}^T \mathbb{P}_1, \quad (5.29)$$

where the relation (5.8) has also been used.

Assume the following forms for  $\boldsymbol{\varepsilon}_{(\mathbf{N}_1)}$  and  $\boldsymbol{\varepsilon}_{(\mathbf{N}_2)}$ :

$$\begin{aligned} \boldsymbol{\varepsilon}_{(\mathbf{N}_1)} &= \mathbf{s}_1 \otimes \mathbf{t}_1 - \mathbf{t}_1 \otimes \mathbf{s}_1 \\ \boldsymbol{\varepsilon}_{(\mathbf{N}_2)} &= \mathbf{s}_2 \otimes \mathbf{t}_2 - \mathbf{t}_2 \otimes \mathbf{s}_2, \end{aligned} \quad (5.30)$$

such that  $\{\mathbf{s}_1, \mathbf{t}_1, \mathbf{N}_1\}$  and  $\{\mathbf{s}_2, \mathbf{t}_2, \mathbf{N}_2\}$  form positively oriented orthonormal basis at  $\mathbf{X}_1 \in S_{t_1}$  and  $\mathbf{X}_2 \in S_{t_2}$ , respectively. Furthermore, let  $\mathbf{t}_1$  and  $\mathbf{t}_2$  be related by the outer equality in (5.26) for some curves  $\Gamma_1 \subset S_{t_1}$  and  $\Gamma_2 \subset S_{t_2}$ , i.e.

$$\mathbf{t}_2 = l^{-1} \mathbf{A}^\pm \mathbf{t}_1, \quad (5.31)$$

where  $l = \frac{du_2}{du_1}$  is the ratio of infinitesimal arc-lengths of  $\Gamma_2$  and  $\Gamma_1$ . Use (5.31) to obtain

$$\mathbf{s}_2 = (\mathbf{t}_2 \times \mathbf{N}_2) = l^{-1} (\mathbf{A}^\pm \mathbf{t}_1 \times \mathbf{N}_2). \quad (5.32)$$

By Nanson's formula (cf. (2.24) and (2.77))

$$\mathbf{N}_2 dA_2 = (\mathbf{A}^\pm)^* \mathbf{N}_1 dA_1 \quad (5.33)$$

or

$$\mathbf{N}_2 = j_A^{-1} (\mathbf{A}^\pm)^* \mathbf{N}_1, \quad (5.34)$$

where  $j_A = \frac{dA_2}{dA_1}$  is the ratio of infinitesimal areas of  $S_{t_2}$  and  $S_{t_1}$ . Equation (5.32) then yields

$$\mathbf{s}_2 = (j_A l)^{-1} (\mathbf{A}^\pm \mathbf{t}_1 \times (\mathbf{A}^\pm)^* \mathbf{N}_1). \quad (5.35)$$

Use  $(\mathbf{A}^\pm)^* \mathbf{N}_1 = (\mathbf{A}^\pm \mathbf{s}_1 \times \mathbf{A}^\pm \mathbf{t}_1)$  and the identity  $\mathbf{g} \times (\mathbf{h} \times \mathbf{g}) = (\mathbf{g} \cdot \mathbf{g})\mathbf{h} - (\mathbf{g} \cdot \mathbf{h})\mathbf{g}$ , where  $\{\mathbf{g}, \mathbf{h}\} \in \mathcal{V}$  are arbitrary, to obtain

$$\mathbf{s}_2 = (j_A l)^{-1} (l^2 \mathbf{A}^\pm \mathbf{s}_1 - l(\mathbf{A}^\pm \mathbf{t}_1 \cdot \mathbf{A}^\pm \mathbf{s}_1) \mathbf{t}_2). \quad (5.36)$$

Thus

$$\mathbf{s}_2 \otimes \mathbf{t}_2 - \mathbf{t}_2 \otimes \mathbf{s}_2 = (j_A)^{-1} (\mathbf{A}^\pm \mathbf{s}_1 \otimes \mathbf{A}^\pm \mathbf{t}_1 - \mathbf{A}^\pm \mathbf{t}_1 \otimes \mathbf{A}^\pm \mathbf{s}_1). \quad (5.37)$$

Use (5.30) to conclude that

$$\boldsymbol{\varepsilon}_{(\mathbf{N}_2)} = (j_A)^{-1} \mathbf{A}^\pm \boldsymbol{\varepsilon}_{(\mathbf{N}_1)} (\mathbf{A}^\pm)^T, \quad (5.38)$$

which can be used to eliminate  $\boldsymbol{\varepsilon}_{(\mathbf{N}_1)}$  from (5.29) to get

$$j_A \llbracket \mathbf{K}_2^{-1} \rrbracket \boldsymbol{\varepsilon}_{(\mathbf{N}_2)} = \boldsymbol{\beta}_{r_1}^T \mathbb{P}_1 (\mathbf{A}^\pm)^T. \quad (5.39)$$

Use the definition (5.8) and take the transpose of equation (5.39). Obtain

$$j_A \mathbb{P}_2 \boldsymbol{\beta}_{r_2} = (\mathbf{A}^\pm) \mathbb{P}_1 \boldsymbol{\beta}_{r_1}. \quad (5.40)$$

Note that  $\mathbf{A}^\pm = \mathbf{K}_2^\pm(\mathbf{K}_1^\pm)^{-1}$  and  $j_A = \frac{j_2^\pm}{j_1^\pm}$ , where  $j_a^\pm$  ( $a = 1, 2$ ) represents the ratio of infinitesimal area elements (of the singular surface) in the reference and the intermediate configuration. Substitute these into (5.40) to get

$$j_2^\pm (\mathbf{K}_2^\pm)^{-1} \mathbb{P}_2 \boldsymbol{\beta}_{r_2} = j_1^\pm (\mathbf{K}_1^\pm)^{-1} \mathbb{P}_1 \boldsymbol{\beta}_{r_1}. \quad (5.41)$$

As a result we define the *true surface dislocation density* as

$$\boldsymbol{\beta}^\pm = j^\pm (\mathbf{K}^\pm)^{-1} \mathbb{P} \boldsymbol{\beta}_r. \quad (5.42)$$

For a superficial  $\boldsymbol{\beta}_r^T$ , i.e.  $\boldsymbol{\beta}_r^T \mathbb{P} = \boldsymbol{\beta}_r^T$ , this reduces to

$$\boldsymbol{\beta}^\pm = j^\pm (\mathbf{K}^\pm)^{-1} \boldsymbol{\beta}_r. \quad (5.43)$$

If in the above analysis, we substitute  $\mathbf{F}$  for  $\mathbf{A}$ , we obtain, instead of (5.41), the following relation

$$\hat{j}^\pm (\mathbf{H}^\pm)^{-1} \mathbb{P}_{(\mathbf{n})} \boldsymbol{\beta}_t = j^\pm (\mathbf{K}^\pm)^{-1} \mathbb{P} \boldsymbol{\beta}_r, \quad (5.44)$$

where  $\hat{j}^\pm$  represents the ratio of infinitesimal area elements (of the singular surface) in the spatial and the intermediate configuration. A relation between referential and spatial surface dislocation densities was also obtained in (5.18), whose equivalence to (5.44) can be proved using a relation of the type (5.38).

*Remark 5.1.3.* Note, that in the incoherent case, the tangential plane (to the surface of singularity) in the reference (or spatial) configuration is mapped into two tangent planes in the intermediate configuration. As a result we have two measures of true surface dislocation density for each  $\mathbf{X} \in T_{S_t}$  (or  $\mathbf{x} \in T_{st}$ ), i.e.  $\boldsymbol{\beta}^\pm$ .

*Remark 5.1.4.* (Geometrically necessary boundaries and incidental dislocation boundaries) Recall Subsection 3.2.3, where the notions of geometrically necessary (GND) and statistically stored (SSD) dislocation densities were introduced. As noted therein, the emergence of the need to divide the total dislocation content into GND and SSD was due to an averaged plastic (or elastic) distortion, with the average being considered over some representative volume element (RVE). The incompatibility in such an average plastic distortion yields GND. On the other hand, as a result of averaging, some microstructural information is invariably lost and is thus accommodated in SSD. Consider now the singular surface  $S_t$  across which  $\mathbf{K}$  is discontinuous and generates a distribution of surface dislocations (via (5.9)). If, however, the plastic distortion  $\mathbf{K}$  is an average quantity, the surface dislocation density (from (5.9)) will result only from the incoherency of the averaged  $\mathbf{K}$ . The dislocation boundary formed out of such a density is termed *geometrically necessary boundary* (GNB). To quantify the lost microstructural information (as a result of averaging) at the boundaries, an additional surface dislocation density will be required (similar to SSD in the bulk), the corresponding boundaries being termed *incidental dislocation boundaries* (IDB). These concepts and their relation to their bulk counterparts have been studied recently by Hughes and her co-authors (see [78] and references therein). The role played by these boundaries in various stages of work hardening is a subject of current interest, of which excellent accounts can be found in the articles by Kuhlmann-Wilsdorf and Mughrabi in [123]. In this thesis, we will neglect the presence of IDB and identify all dislocation boundaries with GNB.

### 5.1.3 Jump in the bulk dislocation density

To obtain a jump in  $\boldsymbol{\alpha}^r$  we start by writing the compatibility condition (cf. (2.69)) for  $\nabla \mathbf{K}^{-1}$  as

$$\llbracket \nabla \mathbf{K}^{-1} \rrbracket = \mathbf{Q} \otimes \mathbf{N} + \nabla^S \llbracket \mathbf{K}^{-1} \rrbracket, \quad (5.45)$$

where  $\mathbf{Q} \in Lin$  is arbitrary. In terms of indicial notation this can be rewritten as<sup>1</sup>

$$\llbracket K_{jl,k}^{-1} \rrbracket = Q_{jl} N_k + \llbracket K_{jl}^{-1} \rrbracket_{,m} \mathbb{P}_{mk}. \quad (5.46)$$

Multiplying (5.46) throughout by  $e_{ikl}$  and using the definition (3.22)<sub>1</sub>, we obtain

$$\llbracket \alpha_{ij}^r \rrbracket = e_{ikl} Q_{jl} N_k + e_{ikl} \llbracket K_{jl}^{-1} \rrbracket_{,m} \mathbb{P}_{mk}. \quad (5.47)$$

On the other hand, the jump in  $K_{jl}^{-1}$  can be expressed in terms of the normal time derivative (cf. (2.59) and (2.60)) of  $\llbracket K_{jl}^{-1} \rrbracket$ . Following (2.72) we get

$$\llbracket K_{jl}^{-1} \rrbracket^\circ = U \llbracket K_{jl,k}^{-1} \rrbracket N_k + \llbracket \dot{K}_{jl}^{-1} \rrbracket, \quad (5.48)$$

where  $^\circ$  denotes the normal time derivative. Substituting (5.46) into (5.48) yields

$$U Q_{jl} = \llbracket K_{jl}^{-1} \rrbracket^\circ - \llbracket \dot{K}_{jl}^{-1} \rrbracket. \quad (5.49)$$

---

<sup>1</sup>Recall from Subsection 2.1.4 that the derivatives on the surface are obtained by first extending the surface field to a small neighborhood near the surface, and then projecting the derivative of the extension back on the surface. We assume that the extension always exists and use the same symbol for the field and its extension (cf. remark 2.1.1). Therefore, wherever in the following discussion, the derivative of a surface quantity appears, for e.g.  $\llbracket K_{jl}^{-1} \rrbracket_{,m}$ , it is implicitly assumed that we are considering the derivative of its extension.

Use this in (5.47) to obtain the jump condition for dislocation density for a moving interface (i.e. for  $U \neq 0$ ):

$$U \llbracket \alpha_{ij}^r \rrbracket = -e_{ikl} \llbracket K_{jl}^{-1} \rrbracket N_k + e_{ikl} \llbracket K_{jl}^{-1} \rrbracket N_k + U e_{ikl} \llbracket K_{jl}^{-1} \rrbracket_{,m} \mathbb{P}_{mk}. \quad (5.50)$$

Therefore, the jump in the bulk dislocation density, across a moving interface, can be obtained from the jumps in plastic distortion and the plastic distortion rate. It follows from either (5.47) or (5.50) that

$$\llbracket \alpha_{ij}^r \rrbracket N_i = e_{ikl} \llbracket K_{jl}^{-1} \rrbracket_{,k} N_i, \quad (5.51)$$

where the identity,  $e_{ikl} N_i N_k = 0$ , has been used. The jump in  $\mathbf{K}^{-1}$  is given in (5.6), which in indicial notation can be written as

$$\llbracket K_{ij}^{-1} \rrbracket = k_i N_j + \beta_{ki}^r \epsilon_{kj}^N. \quad (5.52)$$

The tensor  $\epsilon_{kj}^N$  is the two dimensional permutation symbol given by  $\epsilon_{kj}^N = t_k^1 t_j^2 - t_k^2 t_j^1$ , where  $\{t_k^1, t_k^2\} \in T_{S_t}$  such that  $\{t_k^1, t_k^2, N_l\}$  forms a positively-oriented orthonormal basis. Substituting (5.52) into (5.51), and using  $e_{ikl} N_i N_k = 0$ , we get

$$\llbracket \alpha_{ij}^r \rrbracket N_i = e_{ikl} k_j N_{l,k} N_i + e_{ikl} (\beta_{qj}^r \epsilon_{ql}^N)_{,k} N_i. \quad (5.53)$$

Recall from (2.52)<sub>2</sub>,

$$|\nabla \phi| N_{l,k} = \phi_{,lk} - N_l \phi_{,kn} N_n, \quad (5.54)$$

where  $\phi(\mathbf{X}, t) = 0$  defines the surface  $S_t$  (cf. (2.48)). Multiplying both sides of (5.54) by  $e_{ikl} N_i$  and noting, that  $\phi_{,lk} e_{ikl} = 0$ ,  $e_{ikl} N_i N_l = 0$ , and  $|\nabla \phi| \neq 0$ , we can obtain

$$e_{ikl} N_{l,k} N_i = 0. \quad (5.55)$$



Consequently (5.53) reduces to

$$\begin{aligned} \llbracket \alpha_{ij}^r \rrbracket N_i &= e_{ikl}(\beta_{qj}^r \epsilon_{ql}^N)_{,k} N_i \\ &= \beta_{qj,k}^r e_{ikl} \epsilon_{ql}^N N_i + \beta_{qj}^r e_{ikl} \epsilon_{ql,k}^N N_i, \end{aligned} \quad (5.56)$$

where (5.56)<sub>2</sub> is obtained using the chain rule for differentiation. Note the following two identities:

$$e_{ikl} \epsilon_{ql}^N N_i = \mathbb{P}_{qk}, \quad \text{and} \quad (5.57)$$

$$e_{ikl} \epsilon_{ql,k}^N N_i = 2HN_q, \quad (5.58)$$

where  $H$  is the mean curvature. The relation (5.57) follows from a straightforward calculation using the definition of  $\epsilon_{ql}^N$  and the rules for vector cross product. To obtain (5.58), start by taking a divergence of (5.57) to get

$$e_{ikl} \epsilon_{ql,k}^N N_i + e_{ikl} \epsilon_{ql}^N N_{i,k} = \mathbb{P}_{qk,k}. \quad (5.59)$$

Moreover, using the definition (2.56) of curvature tensor  $L$  (which satisfies  $L = L^T$  and  $LN = \mathbf{0}$ ), we can write the gradient of the normal as  $\nabla \mathbf{N} = -L + (\nabla \mathbf{N})\mathbf{N} \otimes \mathbf{N}$ . We use this and the symmetry of  $L$  to evaluate the second term in (5.59) as

$$\begin{aligned} e_{ikl} \epsilon_{ql}^N N_{i,k} &= e_{ikl} \epsilon_{ql}^N N_{i,p} N_p N_k \\ &= -\mathbb{P}_{qi} N_{i,p} N_p, \end{aligned} \quad (5.60)$$

$$= -N_{q,p} N_p, \quad (5.61)$$

where the equality (5.60) is obtained using (5.57), and the equality (5.61) follows on using the definition  $\mathbb{P}_{qi} = \delta_{qi} - N_q N_i$  and that  $N_{i,p} N_i = 0$ , which is a consequence of  $|\mathbf{N}| = 1$ . On

the other hand, use the definition of  $\mathbb{P}_{qk}$  and the chain rule for differentiation to write

$$\mathbb{P}_{qk,k} = -N_{q,k}N_k - N_qN_{k,k}. \quad (5.62)$$

Substitute (5.61) and (5.62) into (5.59). The relation (5.58) then follows upon noting that  $\text{Div } \mathbf{N} = -2H$  (cf. (2.57) and (2.58)<sub>1</sub>).

Use identities (5.57) and (5.58) to obtain the equivalent form of (5.56) as

$$[[\alpha_{ij}^r]]N_i = \beta_{qj,k}^r \mathbb{P}_{qk} + 2H\beta_{qj}^r N_q \quad (5.63)$$

or in bold notations as  $[[\boldsymbol{\alpha}_r^T]]\mathbf{N} = \text{Div}^S \boldsymbol{\beta}_r^T + 2H\boldsymbol{\beta}_r^T \mathbf{N}$ . To gain further insight into this result, we will use the surface divergence theorem from remark 2.2.1. According to the theorem (cf. (2.105)), for any arbitrary surface  $S \subset S_t$ , we have

$$\oint_{\partial S} \boldsymbol{\beta}_r^T \boldsymbol{\nu} dL = \int_S (\text{Div}^S \boldsymbol{\beta}_r^T + 2H\boldsymbol{\beta}_r^T \mathbf{N}) dA, \quad (5.64)$$

where  $\boldsymbol{\nu}$  is the outer unit normal to  $\partial S$  such that  $(\mathbf{N}, \boldsymbol{\nu}, \mathbf{t})$  form a positively-oriented orthogonal triad at  $\partial S$  with  $\mathbf{t}$  being the tangent vector along  $\partial S$ . Therefore, if  $[[\boldsymbol{\alpha}_r^T]]\mathbf{N} = \mathbf{0}$ , then using (5.63), we obtain from (5.64)

$$\oint_{\partial S} \boldsymbol{\beta}_r^T \boldsymbol{\nu} dL = \mathbf{0}, \quad (5.65)$$

which can be understood as a conservation law for surface dislocations. This can be seen as analogous to the conservation law for  $\boldsymbol{\alpha}_r$ , according to which for any arbitrary volume  $\Omega \subset \kappa_r$  with  $S_t \cap \Omega = \emptyset$ ,

$$\oint_{\partial \Omega} \boldsymbol{\alpha}_r^T \mathbf{N} dA = \mathbf{0}, \quad (5.66)$$

where  $\mathbf{N}$  is the normal to  $\partial \Omega$ . The physical interpretation of (5.66) is that no bulk dislocations can arbitrarily end inside the solid which lacks any surface of discontinuities. The

relation (5.65), on the other hand, provides us with the corresponding interpretation for surface dislocations. Therefore for a vanishing normal jump in  $\boldsymbol{\alpha}_r^T$ , the surface with a dislocation distribution can not end arbitrarily inside the solid. This implies that such a surface will either end at the boundary of the solid or at a surface dislocation node (see remark 5.1.2). If, however,  $[[\boldsymbol{\alpha}_r^T]]\mathbf{N} \neq \mathbf{0}$ , then for  $S = S_t \cap \Omega \neq \emptyset$ , the integral relation (5.66) is of the form

$$\oint_{\partial\Omega} \boldsymbol{\alpha}_r^T \mathbf{N} dA = \int_S [[\boldsymbol{\alpha}_r^T]] \mathbf{N} dA. \quad (5.67)$$

This result follows from the divergence theorem for piecewise smooth fields (2.97), and the conservation law  $\text{Div } \boldsymbol{\alpha}_r^T = \mathbf{0}$ , which holds away from the surface and follows immediately from the definition of  $\boldsymbol{\alpha}_r$ . Finally, combining relations (5.63), (5.64) and (5.68) we obtain the following integral balance law for conservation of dislocations in an arbitrary volume  $\Omega \subset \kappa_r$  such that  $S = S_t \cap \Omega \neq \emptyset$ :

$$\oint_{\partial S} \boldsymbol{\beta}_r^T \boldsymbol{\nu} dL = \oint_{\partial\Omega} \boldsymbol{\alpha}_r^T \mathbf{N} dA. \quad (5.68)$$

*Remark 5.1.5.* The jump in the total dislocation density can be obtained using (3.23) and (2.46):

$$[[\boldsymbol{\alpha}]] = \langle J_K \mathbf{K}^{-1} \rangle [[\boldsymbol{\alpha}_r]] + [[J_K \mathbf{K}^{-1}]] \langle \boldsymbol{\alpha}_r \rangle. \quad (5.69)$$

*Remark 5.1.6.* For continuous  $\mathbf{K}^{-1}$ , (5.50) reduces to

$$U[[\boldsymbol{\alpha}_{ij}^r]] = -e_{ikl} [[K_{jl}^{-1}]] N_k. \quad (5.70)$$

This provides us with a relation, for moving interfaces, between jump in plastic distortion rate and the jump in bulk dislocation density when plastic distortion is continuous across the interface. Such a relation will be used below, in the section on acceleration waves.

## 5.2 Shock waves

Shock waves are defined as moving (i.e.  $U \neq 0$ ) singular surfaces across which the deformation  $\chi$  is continuous but deformation gradient  $\mathbf{F}$  ( $= \nabla\chi$ ) and therefore velocity  $\mathbf{v}$  ( $= \dot{\chi}$ ) is discontinuous. As will be shown below, a non zero jump in  $\mathbf{F}$  is necessary for the existence of shocks, unlike  $\mathbf{H}$  and  $\eta$ , which might or might not be discontinuous. Higher order derivatives of  $\chi$  (for example  $\nabla\mathbf{F}$  or  $\dot{\mathbf{F}}$ ) can also be discontinuous.

Shock waves in elastic plastic solids were first studied by Taylor, von Karman, and Rakhmatoolin (see for e.g. [163, 39, 41]). The plastic deformation, in these works (and in most of the which followed), is understood in a sense that there exists a nonlinear relation between stress and (total) strain, whereas a material is called elastic when this relation is linear. Moreover, the analysis is restricted to one dimension (e.g. a bar with cylindrical section). For a general three dimensional case, however, there are very few analytical results. As we shall point out, this is due to highly complicated nature of the governing equations and also due to the fact that one, in general, is required to integrate the bulk flow rules to obtain state of plastic deformation at the shock [40, 56]. In first two subsections below, we will obtain some general results on the behavior of elastic and plastic shock waves. These results are mostly restricted to shocks of small amplitudes. In the last subsection, however, we take up the case of a plane shock wave, which also coincides with a surface of dislocations. We obtain simple equations, which for given material parameters can be solved for calculating the surface dislocation density and the shock speed. In the next section, we will take up the topic of weak shock waves or acceleration waves, which are analytically tractable and we avoid many difficulties, which otherwise arise in dealing with shock waves.

The kinematical compatibility conditions for a shock wave are given by (cf. (2.65) and (2.73))

$$[[\mathbf{F}]] = \mathbf{a} \otimes \mathbf{N}, \quad \text{and} \quad [[\mathbf{v}]] = -U\mathbf{a}, \quad (5.71)$$

where  $\mathbf{a} \in \mathcal{V}$  is arbitrary, and  $\mathbf{N}$  and  $U$  are the unit normal and the normal velocity field associated with the shock wave, respectively. The jump conditions resulting from the balance of linear momentum and energy were obtained in Subsection 3.4.3. For an adiabatic process they are (cf. (2.144) and (3.89))

$$[[\mathbf{P}]]\mathbf{N} = U^2\rho_\kappa\mathbf{a}, \quad \text{and} \quad U\rho_\kappa[[e]] = U\langle\mathbf{P}\rangle \cdot [[\mathbf{F}]], \quad (5.72)$$

where

$$\rho_\kappa e = J_K^{-1}W(\mathbf{H}, \eta), \quad \mathbf{P} = J_K^{-1}W_{\mathbf{H}}\mathbf{K}^T, \quad \text{and} \quad \rho_\kappa\theta = J_K^{-1}W_\eta. \quad (5.73)$$

Equations (5.71) and (5.72) relate the thermodynamical state  $\mathcal{R}^- = \{\mathbf{F}^-, \mathbf{H}^-, \eta^-\}$  behind the shock to the thermodynamical state  $\mathcal{R}^+ = \{\mathbf{F}^+, \mathbf{H}^+, \eta^+\}$  ahead of the shock. Such relations are called Hugoniot's equations. Denote the set of all states, which for a given  $\mathcal{R}^+$  and  $\mathbf{N}$  satisfy relations (5.71) and (5.72) as  $\mathfrak{R}(\mathcal{R}^+, \mathbf{N})$ . The speed  $U$  in (5.72) can be selected so that  $U \geq 0$ , without loss of any generality. Consider a state  $\mathcal{R} = \{\mathbf{F}, \mathbf{H}, \eta\} \in \mathfrak{R}(\mathcal{R}^+, \mathbf{N})$  such that  $\mathcal{R} \neq \mathcal{R}^+$ . If  $\mathbf{F} \neq \mathbf{F}^+$  then  $U$  can be calculated from (5.72)<sub>1</sub> (multiplying both sides of the equation by  $\mathbf{a}$  and then dividing by  $|\mathbf{a}|$ ), but if  $\mathbf{F} = \mathbf{F}^+$  (with  $\eta \neq \eta^-$  or  $\mathbf{H} \neq \mathbf{H}^-$ ) then  $e(\mathcal{R}) \neq e(\mathcal{R}^+)$  and (5.72)<sub>2</sub> implies that  $U = 0$ . This contradicts the fundamental definition of shock. Therefore, we can conclude that  $\mathbf{F} \neq \mathbf{F}^+$  is a necessary condition for the existence of shocks in solids. For  $\mathcal{R} = \mathcal{R}^+$ , it is evident from equations (5.72) that  $U$  remains undetermined. As will be shown below,  $U$  is then obtained from a characteristic equation. We call the discontinuity described above, a shock, only when  $U \neq 0$ . In addition

to equation (5.72), a shock should also satisfy the second law of thermodynamics in the form (cf. (3.97))

$$-U\rho_\kappa[[\eta]] \geq 0. \quad (5.74)$$

The inequality (5.74) is sometimes used as an admissibility criteria to resolve any non-uniqueness in the solution.

Assume that at a given material point on the shock surface, the state ahead of the shock and the normal  $\mathbf{N}$  are known. The problem is then to determine the state behind the shock and the speed of the shock. These are fourteen unknowns, since the jump  $[[\mathbf{K}^{-1}]]$ , in general, is a full rank tensor (cf. (5.6)). We would therefore need additional relations for a full determination of the state behind the shock. These relations are provided by the constitutive equations for plastic flow. In most of the literature on plastic shock waves, such a constitutive relation is obtained by integrating the flow rule for  $\dot{\mathbf{K}}$ . However, this has been done for the simplest of the flow rules, and integrating general flow rules might prove to be a challenging task. Another possibility is to posit an independent flow rule for  $[[\mathbf{K}^{-1}]]$ , as was suggested by Craggs [40] and Germain & Lee [56]. The basis for such considerations has been ad hoc in nature and no experimental data seems to be available to support it. Even after assuming a constitutive law, obtaining solutions for admissible shock waves remains a difficult task (in the full three dimensional theory) because of the highly non-linear nature of equations (5.72). Below we will obtain some results valid only for states in a small neighborhood of  $\mathcal{R}^+$ . For an elastic shock wave, we follow Šilhavý ([156], Ch. 23) to show that the jump in entropy is of the third order in deformation gradient and that entropy and speed  $U$  are strictly increasing functions in the neighborhood of  $\mathcal{R}^+$ . Next,

we will re-evaluate these claims for plastic shock waves and show that the jump in entropy across the shock is now of the first order in plastic distortion. Further, we will show that the monotonicity of  $U$  will now depend on the constitutive structure for plastic flow. In Subsection 5.2.3, however, we take a different stand and look at the problem of shock wave as a dislocation wall. We calculate the surface dislocation distribution at a shock assuming that  $\mathbf{a}$  and  $U$  are known (in addition to the state ahead of the shock).

For the purpose of next two subsections, we consider curves in  $\mathfrak{R}(\mathcal{R}^+, \mathbf{N})$ , parameterized by  $\tau \in \mathbb{R}$  such that any point on the curve is given by  $\mathcal{R}(\tau) = \{\mathbf{F}(\tau), \mathbf{H}(\tau), \eta(\tau)\} \in \mathfrak{R}(\mathcal{R}^+, \mathbf{N})$ . Furthermore, we require that  $\mathcal{R}(0) = \mathcal{R}^+$  and  $\mathcal{R}(\tau) \neq \mathcal{R}^+$  for  $\tau \neq 0$ . In the following subsections we will, in particular, be interested in the behavior of the shock for  $\tau$  close to zero. As discussed above, the shock speed does not necessarily tends to zero as  $\tau$  approaches zero. Let  $U_0 = \lim_{\tau \rightarrow 0} U(\tau)$  and  $\mathbf{e} = \lim_{\tau \rightarrow 0} \dot{\mathbf{a}}(\tau)$ . Here and in next two subsections,  $(\dot{\phantom{x}})$  denotes the derivative along the curve, with  $(\dot{\phantom{x}})(0)$  the value as  $\tau$  approaches zero (thus  $\mathbf{e} = \dot{\mathbf{a}}(0)$ ).

### 5.2.1 Elastic shock wave

In this subsection, we will show that for an elastic shock wave, the jump in entropy is of the third order in the jump in deformation gradient and that both  $\eta$  and  $U$  are strictly increasing functions of  $\tau$  near  $\tau = 0$ . We define a shock wave to be elastic when  $[[\mathbf{K}^{-1}]] = \mathbf{0}$  (which implies  $\dot{\mathbf{K}}(\tau) = \mathbf{0}$ ). Therefore,

$$\dot{\mathbf{H}}(\tau) = \dot{\mathbf{F}}(\tau)\mathbf{K} = -\dot{\mathbf{a}}(\tau) \otimes \mathbf{K}^T \mathbf{N}, \quad (5.75)$$

where (5.75)<sub>1</sub> and (5.75)<sub>2</sub> follow from (3.18) and (5.71)<sub>1</sub>, respectively. Differentiate (5.72)<sub>2</sub> with respect to  $\tau$  and obtain

$$-J_K^{-1} \left\{ W_{\mathbf{H}} \cdot \dot{\mathbf{H}} + W_{\eta} \dot{\eta} \right\} = \frac{1}{2} \dot{\mathbf{P}} \mathbf{N} \cdot \mathbf{a} + \langle \mathbf{P} \rangle \mathbf{N} \cdot \dot{\mathbf{a}}, \quad (5.76)$$

which on using (5.73) reduces to

$$-\rho_{\kappa} \theta \dot{\eta} = \frac{1}{2} \dot{\mathbf{P}} \mathbf{N} \cdot \mathbf{a} + \frac{1}{2} \llbracket \mathbf{P} \rrbracket \mathbf{N} \cdot \dot{\mathbf{a}}. \quad (5.77)$$

Evaluating (5.77) at  $\tau = 0$ , and noting that  $\mathbf{a}(0) = \mathbf{0}$ ,  $\dot{\mathbf{a}}(0) = \mathbf{e}$ , and  $\theta > 0$ , we get

$$\dot{\eta}(0) = 0. \quad (5.78)$$

Differentiating (5.77) with respect to  $\tau$ , and recalling that  $\dot{\rho}_{\kappa} = 0$  from mass balance, yields

$$-\rho_{\kappa} \dot{\theta} \dot{\eta} - \rho_{\kappa} \theta \ddot{\eta} = \frac{1}{2} \ddot{\mathbf{P}} \mathbf{N} \cdot \mathbf{a} + \frac{1}{2} \llbracket \mathbf{P} \rrbracket \mathbf{N} \cdot \ddot{\mathbf{a}}, \quad (5.79)$$

which at  $\tau = 0$  gives us

$$\ddot{\eta}(0) = 0. \quad (5.80)$$

Differentiate (5.79) and evaluate it at  $\tau = 0$  to obtain

$$-\rho_{\kappa} \theta_0 \ddot{\eta}(0) = \frac{1}{2} \ddot{\mathbf{P}}(0) \mathbf{N} \cdot \mathbf{e} - \frac{1}{2} \dot{\mathbf{P}}(0) \mathbf{N} \cdot \ddot{\mathbf{a}}(0), \quad (5.81)$$

where  $\theta_0 = \theta(0)$ . On the other hand, differentiating (5.72)<sub>1</sub> yields

$$-\dot{\mathbf{P}} \mathbf{N} = 2\rho_{\kappa} U \dot{U} \mathbf{a} + \rho_{\kappa} U^2 \dot{\mathbf{a}}. \quad (5.82)$$

Recalling the constitutive structure of  $\mathbf{P}$  and using the chain rule for differentiation we can write

$$\dot{\mathbf{P}} = \mathbf{P}_{\mathbf{H}}[\dot{\mathbf{H}}] + \mathbf{P}_{\eta} \dot{\eta}. \quad (5.83)$$



At  $\tau = 0$ , use (5.75)<sub>2</sub> and (5.78), to conclude that  $\dot{\mathbf{P}}(0) = -\mathbf{P}_{\mathbf{H}}(0)[\mathbf{e} \otimes \mathbf{K}^T \mathbf{N}]$ , using which we can obtain from (5.82)

$$\mathbf{P}_{\mathbf{H}}(0)[\mathbf{e} \otimes \mathbf{K}^T \mathbf{N}] \mathbf{N} = \rho_{\kappa} U_0^2 \mathbf{e}. \quad (5.84)$$

Substituting  $\mathbf{P}$  from (5.73)<sub>2</sub>, equation (5.84) reduces to the familiar form of the characteristic equation:

$$J_K^{-1} W_{\mathbf{H}\mathbf{H}}(0)[\mathbf{e} \otimes \mathbf{K}^T \mathbf{N}] \mathbf{K}^T \mathbf{N} = \rho_{\kappa} U_0^2 \mathbf{e}. \quad (5.85)$$

This implies that  $U_0^2 \geq 0$  if and only if  $W_{\mathbf{H}\mathbf{H}}$  satisfies Legendre-Hadamard condition at  $\tau = 0$ , i.e.

$$W_{\mathbf{H}\mathbf{H}}(0)[\mathbf{e} \otimes \mathbf{K}^T \mathbf{N}, \mathbf{e} \otimes \mathbf{K}^T \mathbf{N}] \geq 0, \quad (5.86)$$

which is also equivalent to satisfying hyperbolicity condition at  $\tau = 0$ . Before we move ahead, it is important to note that the form of characteristic equation above is similar to the one obtained for elastic acceleration waves (see Subsection 5.3.1), and therefore we can conclude that shock wave speed approaches the acceleration wave speed as  $\tau \rightarrow 0$ , but as we will see below, the shock wave speed increases monotonically with  $\tau$  near  $\tau = 0$ .

Differentiating (5.83) one more time, and evaluate it at  $\tau = 0$  to get

$$-\ddot{\mathbf{P}}(0) \mathbf{N} = 4\rho_{\kappa} U_0 \dot{U}(0) \mathbf{e} + \rho_{\kappa} U_0^2 \ddot{\mathbf{a}}(0). \quad (5.87)$$

Substitute this in (5.81) and use (5.82) (at  $\tau = 0$ ). Obtain

$$\begin{aligned} -\rho_{\kappa} \theta_0 \ddot{\eta}(0) &= \frac{1}{2} \ddot{\mathbf{P}}(0) \mathbf{N} \cdot \mathbf{e} - \frac{1}{2} \dot{\mathbf{P}}(0) \mathbf{N} \cdot \ddot{\mathbf{a}}(0) \\ &= -2\rho_{\kappa} U_0 \dot{U}(0) - \frac{1}{2} \rho_{\kappa} U_0^2 \ddot{\mathbf{a}}(0) \cdot \mathbf{e} + \frac{1}{2} \rho_{\kappa} U_0^2 \mathbf{e} \cdot \ddot{\mathbf{a}}(0) \\ &= -2\rho_{\kappa} U_0 \dot{U}(0) \end{aligned} \quad (5.88)$$

and since  $\rho_\kappa > 0$ , we have

$$\theta_0 \ddot{\eta}(0) = 2U_0 \dot{U}(0). \quad (5.89)$$

Differentiating (5.83) at  $\tau = 0$ , yields

$$\ddot{\mathbf{P}}(0) = -\mathbf{P}_{\mathbf{H}}(0)[\ddot{\mathbf{a}}(0) \otimes \mathbf{K}^T \mathbf{N}] + \mathbf{P}_{\mathbf{HH}}(0)[\mathbf{e} \otimes \mathbf{K}^T \mathbf{N}, \mathbf{e} \otimes \mathbf{K}^T \mathbf{N}], \quad (5.90)$$

where we have used equations (5.78) and (5.80) to eliminate  $\dot{\eta}(0)$  and  $\ddot{\eta}(0)$ . Multiply (5.90) throughout by  $\mathbf{e} \otimes \mathbf{N}$  and use (5.73)<sub>2</sub> to obtain

$$\begin{aligned} \ddot{\mathbf{P}}(0) \mathbf{N} \cdot \mathbf{e} &= -J_K^{-1} W_{\mathbf{HH}}(0)[\ddot{\mathbf{a}}(0) \otimes \mathbf{K}^T \mathbf{N}] \cdot (\mathbf{e} \otimes \mathbf{K}^T \mathbf{N}) \\ &+ J_K^{-1} W_{\mathbf{HHH}}(0)[\mathbf{e} \otimes \mathbf{K}^T \mathbf{N}, \mathbf{e} \otimes \mathbf{K}^T \mathbf{N}, \mathbf{e} \otimes \mathbf{K}^T \mathbf{N}], \end{aligned} \quad (5.91)$$

which on using the symmetry of  $W_{\mathbf{HH}}$  and (5.85) reduces to

$$\ddot{\mathbf{P}}(0) \mathbf{N} \cdot \mathbf{e} = -\rho_\kappa U_0^2 \mathbf{e} \cdot \ddot{\mathbf{a}}(0) + J_K^{-1} W_{\mathbf{HHH}}(0)[\mathbf{e} \otimes \mathbf{K}^T \mathbf{N}, \mathbf{e} \otimes \mathbf{K}^T \mathbf{N}, \mathbf{e} \otimes \mathbf{K}^T \mathbf{N}], \quad (5.92)$$

Taking a dot product of (5.87) with  $\mathbf{e}$  and substituting from (5.92) we obtain

$$4\rho_\kappa U_0 \dot{U}(0) = -J_K^{-1} W_{\mathbf{HHH}}(0)[\mathbf{e} \otimes \mathbf{K}^T \mathbf{N}, \mathbf{e} \otimes \mathbf{K}^T \mathbf{N}, \mathbf{e} \otimes \mathbf{K}^T \mathbf{N}]. \quad (5.93)$$

Combining this with (5.89) we see that  $\ddot{\eta}(0)$  is at least of the third order in  $\mathbf{e}$ , i.e.

$$2\rho_\kappa \theta_0 \ddot{\eta}(0) = -J_K^{-1} W_{\mathbf{HHH}}(0)[\mathbf{e} \otimes \mathbf{K}^T \mathbf{N}, \mathbf{e} \otimes \mathbf{K}^T \mathbf{N}, \mathbf{e} \otimes \mathbf{K}^T \mathbf{N}]. \quad (5.94)$$

For a genuinely nonlinear characteristic field  $(U_0, \mathbf{e})$

$$W_{\mathbf{HHH}}(0)[\mathbf{e} \otimes \mathbf{K}^T \mathbf{N}, \mathbf{e} \otimes \mathbf{K}^T \mathbf{N}, \mathbf{e} \otimes \mathbf{K}^T \mathbf{N}] \neq 0. \quad (5.95)$$

This definition of nonlinearity has been provided by Šilhavý ([156], Section 23.2), who has motivated it from the work on shock waves by Lax ([101], [102]). Lax found a similar

condition to be necessary for the emergence of shock waves in a solution to a nonlinear differential equation. Note that the condition (5.95) excludes linear elasticity, since we then have  $W_{\mathbf{H}\mathbf{H}\mathbf{H}} = \mathbf{0}$ . For a genuinely nonlinear characteristic field, it follows from (5.89) that  $\ddot{\eta}(0)$  and  $\dot{U}(0)$  have same sign (assuming  $U > 0$ ) and arbitrariness in the sign of  $\tau$  can be used to conclude that both  $\eta$  and  $U$  are monotonically increasing functions of  $\tau$  near  $\tau = 0$ . Finally, differentiate (5.74) thrice with respect to  $\tau$ , evaluating it at  $\tau = 0$ , and using (5.78) and (5.80), we can obtain (for  $\rho_\kappa > 0$ ,  $U_0 > 0$ ,  $\theta_0 > 0$ , and  $J_K > 0$ )

$$W_{\mathbf{H}\mathbf{H}\mathbf{H}}(0)[\mathbf{e} \otimes \mathbf{K}^T \mathbf{N}, \mathbf{e} \otimes \mathbf{K}^T \mathbf{N}, \mathbf{e} \otimes \mathbf{K}^T \mathbf{N}] \leq 0 \quad (5.96)$$

which can be seen as a constitutive restriction. In one dimension, this condition restricts the stress strain curve to be downward convex for compressive shock waves.<sup>2</sup>

### 5.2.2 Plastic shock wave

In the following discussion on plastic shock waves we will, in particular, show that the jump in entropy is now of the first order in the jump in deformation gradient (for fixed  $\dot{\mathbf{K}}(0)$ ). The jump in entropy is also of the first order in the jump in plastic distortion. Furthermore, unlike elastic shock waves,  $\dot{\eta}(0)$  and  $\dot{U}(0)$  are no more of the same sign, and to make any judgements regarding monotonicity of  $U$  near  $\tau = 0$  will require further constitutive knowledge. Another deviation from elastic shock waves is that we no more require hyperbolicity in the sense of (5.86) as a necessary condition for the existence of waves.

---

<sup>2</sup>The paper by Weyl [175] should be mentioned in this regard, who obtained such conditions for fluids.

In the context of one dimensional elasticity, see [34] and [133].

For a plastic shock wave  $\dot{\mathbf{K}}(\tau) \neq \mathbf{0}$ , and therefore we have, instead of (5.75)

$$\dot{\mathbf{H}}(\tau) = \dot{\mathbf{F}}\mathbf{K} + \mathbf{F}\dot{\mathbf{K}} = -\dot{\mathbf{a}} \otimes \mathbf{K}^T \mathbf{N} + \mathbf{F}\dot{\mathbf{K}}. \quad (5.97)$$

Differentiate (5.72)<sub>2</sub> with respect to  $\tau$ , and use (5.73)<sub>2</sub> to get

$$-\rho_\kappa \theta \dot{\eta} + \mathbf{E} \cdot \dot{\mathbf{K}}\mathbf{K}^{-1} = \frac{1}{2} \dot{\mathbf{P}}\mathbf{N} \cdot \mathbf{a} + \frac{1}{2} \llbracket \mathbf{P} \rrbracket \mathbf{N} \cdot \dot{\mathbf{a}}, \quad (5.98)$$

where  $\mathbf{E} = (J_K^{-1}W\mathbf{1} - \mathbf{F}^T\mathbf{P})$  is the Eshelby tensor. For  $\tau = 0$ , it follows from (5.98) that

$$\rho_\kappa \theta_0 \dot{\eta}(0) = \mathbf{E}_0 \cdot \dot{\mathbf{K}}_0 \mathbf{K}_0^{-1}, \quad (5.99)$$

where  $(\cdot)_0 \equiv (\cdot)(0)$ . Therefore, the jump in specific entropy is of the first order in the jump in plastic distortion. To evaluate the second order term, differentiate (5.98) again at  $\tau = 0$ .

Obtain

$$-\rho_\kappa \dot{\theta}(0) \dot{\eta}(0) - \rho_\kappa \theta_0 \ddot{\eta}(0) + \dot{\mathbf{E}}_0 \cdot \dot{\mathbf{K}}_0 \mathbf{K}_0^{-1} + \mathbf{E}_0 \cdot \ddot{\mathbf{K}}_0 \mathbf{K}_0^{-1} - \mathbf{E}_0 \cdot (\dot{\mathbf{K}}_0 \mathbf{K}_0^{-1})^2 = 0. \quad (5.100)$$

Using the definition of  $\mathbf{E}$  we can write,

$$\begin{aligned} \dot{\mathbf{E}} &= -J_K^{-1}W(\text{tr} \dot{\mathbf{K}}\mathbf{K}^{-1})\mathbf{1} + J_K^{-1}\dot{W}\mathbf{1} - \dot{\mathbf{F}}^T\mathbf{P} - \mathbf{F}^T\dot{\mathbf{P}} \\ &= -(\mathbf{E} \cdot \dot{\mathbf{K}}\mathbf{K}^{-1})\mathbf{1} + \rho_\kappa \theta \dot{\eta}\mathbf{1} + (\mathbf{P}^T \dot{\mathbf{a}} \otimes \mathbf{N}) - (\dot{\mathbf{a}} \cdot \mathbf{P}\mathbf{N})\mathbf{1} - \mathbf{F}^T\dot{\mathbf{P}}, \end{aligned} \quad (5.101)$$

where the second equality has been obtained using (5.73)<sub>2,3</sub> and (5.97). At  $\tau = 0$ , (5.101) reduces to (using (5.99))

$$\dot{\mathbf{E}}_0 = (\mathbf{P}_0^T \mathbf{e} \otimes \mathbf{N}) - (\mathbf{e} \cdot \mathbf{P}_0 \mathbf{N})\mathbf{1} - \mathbf{F}_0^T \dot{\mathbf{P}}_0. \quad (5.102)$$

On the other hand, differentiate (5.73)<sub>2,3</sub> to get

$$\rho_\kappa \dot{\theta} = -\rho_\kappa \theta (\text{tr} \dot{\mathbf{K}}\mathbf{K}^{-1}) + J_K^{-1}W_{\eta\eta}\dot{\eta} + J_K^{-1}W_{\eta\mathbf{H}} \cdot \dot{\mathbf{H}} \quad \text{and} \quad (5.103)$$

$$\dot{\mathbf{P}} = -(\text{tr} \dot{\mathbf{K}}\mathbf{K}^{-1})\mathbf{P} + J_K^{-1}W_{\mathbf{H}\mathbf{H}}[\dot{\mathbf{H}}]\mathbf{K}^T + J_K^{-1}\dot{\eta}W_{\mathbf{H}\eta}\mathbf{K}^T + J_K^{-1}W_{\mathbf{H}}\dot{\mathbf{K}}^T, \quad (5.104)$$

respectively. Use (5.97) and (5.99) to write these at  $\tau = 0$  in the following form:

$$\rho_\kappa \dot{\theta}_0 = \mathbf{A} \cdot \dot{\mathbf{K}}_0 + \mathbf{d} \cdot \mathbf{e} \quad (5.105)$$

$$\dot{\mathbf{P}}_0 = -J_{K_0}^{-1} W_{\mathbf{H}\mathbf{H}}^0 [\mathbf{e} \otimes \mathbf{K}_0^T \mathbf{N}] \mathbf{K}_0^T + \mathcal{A}[\dot{\mathbf{K}}_0], \quad (5.106)$$

where

$$\begin{aligned} \mathbf{A} &= -\rho_\kappa \theta_0 \mathbf{K}_0^{-T} + \frac{J_{K_0}^{-1} W_{\eta\eta}^0}{\rho_\kappa \theta_0} \mathbf{E}_0 \mathbf{K}_0^{-T} + J_{K_0}^{-1} \mathbf{F}_0^T W_{\eta\mathbf{H}}^0, \\ \mathbf{d} &= -J_{K_0}^{-1} W_{\eta\mathbf{H}}^0 \mathbf{K}_0^T \mathbf{N}, \quad \text{and} \\ \mathcal{A}_{ijmn} &= -P_{ij}^0 (K_{ij}^{-1})_0 + J_{K_0}^{-1} (W_{\mathbf{H}\mathbf{H}}^0)_{ipqn} F_{qm}^0 K_{jp}^0 + \frac{J_{K_0}^{-1}}{\rho_\kappa \theta_0} (W_{\eta\mathbf{H}}^0)_{ip} K_{jp}^0 E_{mq}^0 (K_{nq}^{-1})_0 \\ &\quad + J_{K_0}^{-1} (W_{\mathbf{H}}^0)_{in} \delta_{jm}. \end{aligned} \quad (5.107)$$

In the above expressions, we have moved subscript  $_0$  to a superscript whenever there were too many subscripts already. Substituting (5.99), (5.102), (5.105) and (5.106) into (5.100) we can note that  $\ddot{\eta}(0)$  is linear in  $\ddot{\mathbf{K}}_0$ , quadratic in  $\dot{\mathbf{K}}_0$  and linear in  $\dot{\mathbf{K}}_0 \otimes \mathbf{e}$ . Therefore, for fixed  $\dot{\mathbf{K}}_0$ , the jump in entropy is of the first order in the jump in deformation gradient. This is a first major departure from elastic shock waves. We next demonstrate the second major departure, where we no more require a hyperbolic condition for the existence of shock waves.

Differentiate (5.72)<sub>1</sub> at  $\tau = 0$  and use (5.106) to obtain

$$J_K^{-1} W_{\mathbf{H}\mathbf{H}}^0 [\mathbf{e} \otimes \mathbf{K}^T \mathbf{N}] \mathbf{K}^T \mathbf{N} - \mathcal{A}[\dot{\mathbf{K}}_0] \mathbf{N} = \rho_\kappa U_0^2 \mathbf{e}. \quad (5.108)$$

This equation replaces (5.85) for plastic shock waves. To solve this equation for  $U_0$  and  $\mathbf{e}$ , we will require a flow rule for  $\dot{\mathbf{K}}_0$ . It is unclear on how should such flow rules be formulated, unless we identify  $\tau$  with the time variable. However in doing so, (5.108) resembles the

characteristic equation for plastic acceleration waves (cf. Subsection 5.3.2). As it is clear from (5.108), it is no more sufficient to have hyperbolicity condition such as (5.86) to ensure that  $U_0^2 \geq 0$ . Finally, to evaluate  $\dot{U}_0$ , differentiate (5.72)<sub>1</sub> twice at  $\tau = 0$  and multiply throughout by  $\mathbf{e}$ . Obtain

$$-\ddot{\mathbf{P}}_0 \mathbf{N} \cdot \mathbf{e} = 4\rho_\kappa U_0 \dot{U}_0 + \rho_\kappa U_0^2 \ddot{\mathbf{a}}_0 \cdot \mathbf{e}, \quad (5.109)$$

where  $\ddot{\mathbf{P}}_0$  can be calculated by differentiating (5.104) at  $\tau = 0$ . This will result in a very lengthy expression for  $\dot{U}_0$ . Avoiding these cumbersome calculations, we can still conclude, just by observation, that unlike elastic shock waves  $\dot{U}_0$  no more has the sign as  $\dot{\eta}_0$  and furthermore to investigate behavior of  $U$  near  $\tau = 0$  will require us to know more about the plastic evolution at the shock. As we shall see, the situation is much simpler in the case of acceleration waves, where it is straightforward to obtain a set of simultaneous equations which can be solved to obtain the state behind the shock.

### 5.2.3 Shock wave as a dislocation wall

In 1958 Smith [158] reported several experimental studies of shock fronts in metals. Motivated by the findings, he concluded that the shock front is an interface with (surface) dislocation distribution (dislocation wall) on the shock surface, remain on the surface through out the propagation of the shock, leaving the bulk without any defects. This model was, however, extended subsequently, notably by Meyers ([117], Ch. 14) and Weertman [173], who argued that the original model of Smith would require excessively high energy for a dislocation wall to move at supersonic speeds. Both Meyers and Weertman allow for plastic deformation to take place in the wake of the shock, thereby avoiding many

shortcomings of Smith's model.

Our aim, in this subsection, is obtain the surface dislocation density and the shock speed which, given  $\mathbf{N}$ ,  $\mathbf{a}$ , and  $[[\eta]]$ , satisfy Hugoniot relations (5.72). Let  $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\} \in \mathcal{V}$  be a fixed orthonormal basis, and assume the shock interface to be plane, with uniform normal  $\mathbf{N} = \mathbf{e}_3$ . The state ahead of the shock is assumed to be given as:  $\mathbf{F}^+ = \mathbf{1}$ ,  $\mathbf{H}^+ = \mathbf{1}$  and  $\eta^+$ . The state behind the shock is denoted by  $\mathcal{R} = \{\mathbf{F}, \mathbf{H}, \eta\} \in \mathfrak{R}(\mathcal{R}^+, \mathbf{N})$ . Consider a uniaxial deformation field such that  $[[\mathbf{F}]] = a\mathbf{e}_3 \otimes \mathbf{e}_3$  with  $a \in \mathbb{R} \setminus \{0, 1\}$ . Thus

$$\mathbf{F} = \mathbf{1} - a\mathbf{e}_3 \otimes \mathbf{e}_3. \quad (5.110)$$

The first Piola stress  $\mathbf{P}$  is related to the second Piola stress  $\mathbf{S}$  by (cf. (3.68) and (3.100))

$$\mathbf{P} = J_K^{-1} \mathbf{H} \mathbf{S} \mathbf{K}^T. \quad (5.111)$$

Considering constitutive relations such that for  $\mathbf{H}^+ = \mathbf{1}$ , we have  $\mathbf{P}^+ = \mathbf{0}$  and  $W^+ = 0$ , Hugoniot relations (5.72) reduce to

$$-J_K^{-1} \mathbf{H} \mathbf{S} \mathbf{K}^T \mathbf{e}_3 = U^2 \rho_\kappa a \mathbf{e}_3, \quad \text{and} \quad -W = \frac{a}{2} \mathbf{H} \mathbf{S} \mathbf{K}^T \mathbf{e}_3 \cdot \mathbf{e}_3. \quad (5.112)$$

Equation (5.112)<sub>2</sub>, on using (5.112)<sub>1</sub>, can also be written as

$$W = \frac{1}{2} \rho_\kappa J_K a^2 U^2. \quad (5.113)$$

We will use equations (5.112) and (5.113) to determine the shock speed and the density of surface dislocations from a given strain energy function and amplitude  $a$ . Our attention will be restricted to the case of small elastic strains, such that the strain energy is given by  $W = \frac{1}{2} \mathbb{C} \boldsymbol{\epsilon} \cdot \boldsymbol{\epsilon}$ , where  $\mathbb{C} = \mathbb{C}(\eta)$  is the elastic modulus<sup>3</sup> and the elastic strain tensor  $\boldsymbol{\epsilon}$  is

<sup>3</sup>The dependence of energy on entropy is only through  $\mathbb{C}$ .

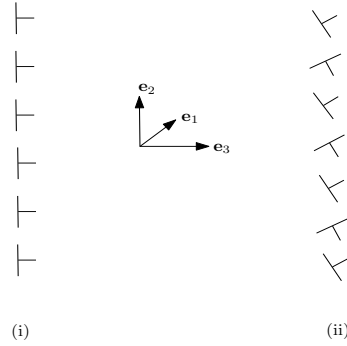


Figure 5.1: Dislocation Walls.<sup>4</sup>

related to  $\mathbf{H}$  as

$$\boldsymbol{\epsilon} = \frac{1}{2}(\mathbf{H}^T \mathbf{H} - \mathbf{1}). \tag{5.114}$$

The second Piola stress is given by  $\mathbf{S} = \text{Sym}W_{\boldsymbol{\epsilon}}$  (cf. (3.101)).

Assume that the plastic flow at the shock interface is governed solely by surface dislocations. This implies that  $[[\mathbf{K}^{-1}]]$  is superficial, i.e.  $[[\mathbf{K}^{-1}]]\mathbb{P} = [[\mathbf{K}^{-1}]]$  or  $\mathbf{k} = \mathbf{0}$  in (5.6).

The state of plastic distortion behind the shock then takes the form (cf. (5.6))

$$\mathbf{K}^{-1} = \mathbf{1} + \boldsymbol{\beta}_r^T \boldsymbol{\varepsilon}_{(\mathbf{N})}, \tag{5.115}$$

where  $\boldsymbol{\varepsilon}_{(\mathbf{N})} = \mathbf{e}_1 \otimes \mathbf{e}_2 - \mathbf{e}_2 \otimes \mathbf{e}_1$ . We now consider two kind of dislocation surfaces, as illustrated in figure 5.1, and discuss these cases separately in the following:

**Case (i)** Consider the dislocation wall of type (i) in figure 5.1. The surface dislocation density is of the form

$$\boldsymbol{\beta}_r^T = \beta \mathbf{e}_2 \otimes \mathbf{e}_1, \tag{5.116}$$

---

<sup>4</sup>These arrays of dislocations should be considered as smeared over the interface, rather than discrete set of individual dislocations.



where  $\beta \in \mathbb{R}$ . Using this we can obtain an expression for the plastic distortion behind the shock from (5.115) as

$$\mathbf{K}^{-1} = \mathbf{1} + \beta \mathbf{e}_2 \otimes \mathbf{e}_2, \quad (5.117)$$

which can be inverted to get<sup>5</sup> (for  $\beta \neq -1$ )

$$\mathbf{K} = \mathbf{1} - \hat{\beta} \mathbf{e}_2 \otimes \mathbf{e}_2, \quad (5.118)$$

where  $\hat{\beta} = \frac{\beta}{1+\beta}$ . The elastic distortion  $\mathbf{H}$  can be then obtained by substituting equations (5.110) and (5.118) in (3.18). We obtain

$$\mathbf{H} = \mathbf{1} - \hat{\beta} \mathbf{e}_2 \otimes \mathbf{e}_2 - a \mathbf{e}_3 \otimes \mathbf{e}_3 \quad (5.119)$$

and therefore the elastic strain tensor, defined in (5.114), is

$$\boldsymbol{\epsilon} = \frac{1}{2} \left\{ (\hat{\beta}^2 - 2\hat{\beta}) \mathbf{e}_2 \otimes \mathbf{e}_2 + (a^2 - 2a) \mathbf{e}_3 \otimes \mathbf{e}_3 \right\}. \quad (5.120)$$

Using (5.118), Hugoniot relations (5.112) become

$$\mathbf{S} \mathbf{e}_3 = (\hat{\beta} - 1) U^2 \rho_\kappa a \mathbf{H}^{-1} \mathbf{e}_3, \quad \text{and} \quad -W = \frac{a}{2} \mathbf{S} \mathbf{e}_3 \cdot \mathbf{H}^T \mathbf{e}_3. \quad (5.121)$$

It follows from (3.18), that  $\mathbf{H}^{-1} = \mathbf{K}^{-1} \mathbf{F}^{-1}$ . The tensor  $\mathbf{K}^{-1}$  is given in (5.117) and  $\mathbf{F}^{-1}$  can be obtained from (5.110) as

$$\mathbf{F}^{-1} = \mathbf{1} + \frac{a}{1-a} \mathbf{e}_3 \otimes \mathbf{e}_3. \quad (5.122)$$

Thus

$$\mathbf{H}^{-1} = \mathbf{1} + \beta \mathbf{e}_2 \otimes \mathbf{e}_2 + \frac{a}{1-a} \mathbf{e}_3 \otimes \mathbf{e}_3 \quad (5.123)$$

---

<sup>5</sup>For arbitrary  $\mathbf{A} \in \text{InvLin}$  and  $\{\mathbf{p}, \mathbf{q}\} \in \mathcal{V}$ ,  $(\mathbf{A} + \mathbf{p} \otimes \mathbf{q})^{-1} = \mathbf{A}^{-1} - (1 + \mathbf{A}^{-1} \mathbf{p} \cdot \mathbf{q})^{-1} (\mathbf{A}^{-1} \mathbf{p} \otimes \mathbf{A}^{-T} \mathbf{q})$ , assuming that  $(1 + \mathbf{A}^{-1} \mathbf{p} \cdot \mathbf{q}) \neq 0$ .

and consequently (5.121)<sub>1</sub> yields

$$\mathbf{S}\mathbf{e}_3 = (\hat{\beta} - 1)U^2\rho_\kappa\frac{a}{1-a}\mathbf{e}_3. \quad (5.124)$$

Relation (5.121)<sub>2</sub>, on the other hand, reduces to (using (5.119))

$$W = \frac{1}{2}a(a-1)\mathbf{S}\mathbf{e}_3 \cdot \mathbf{e}_3. \quad (5.125)$$

To obtain a closed form solution, we assume linear elastic response. For isotropic and cubic symmetry groups, we have constitutive relations (cf. (3.124) and (3.118))

$$W = \frac{1}{2}\lambda(\text{tr } \boldsymbol{\epsilon})^2 + \mu\boldsymbol{\epsilon} \cdot \boldsymbol{\epsilon} \quad , \quad \mathbf{S} = \lambda(\text{tr } \boldsymbol{\epsilon})\mathbf{1} + 2\mu\boldsymbol{\epsilon} \quad (5.126)$$

and

$$\begin{aligned} W &= \frac{1}{2}C_1(\epsilon_{11} + \epsilon_{22} + \epsilon_{33})^2 + C_2(\epsilon_{11}\epsilon_{22} + \epsilon_{11}\epsilon_{33} + \epsilon_{22}\epsilon_{33}) + C_3(\epsilon_{12}^2 + \epsilon_{13}^2 + \epsilon_{23}^2), \\ \mathbf{S} &= C_1(\text{tr } \boldsymbol{\epsilon})\mathbf{1} + C_2[(\epsilon_{22} + \epsilon_{33})\mathbf{e}_1 \otimes \mathbf{e}_1 + (\epsilon_{11} + \epsilon_{33})\mathbf{e}_2 \otimes \mathbf{e}_2 + (\epsilon_{11} + \epsilon_{22})\mathbf{e}_3 \otimes \mathbf{e}_3] \\ &\quad + C_3[\epsilon_{12}(\mathbf{e}_1 \otimes \mathbf{e}_2 + \mathbf{e}_2 \otimes \mathbf{e}_1) + \epsilon_{13}(\mathbf{e}_1 \otimes \mathbf{e}_3 + \mathbf{e}_3 \otimes \mathbf{e}_1) + \epsilon_{23}(\mathbf{e}_2 \otimes \mathbf{e}_3 + \mathbf{e}_3 \otimes \mathbf{e}_2)], \end{aligned} \quad (5.127)$$

respectively, where  $\lambda$ ,  $\mu$ ,  $C_1$ ,  $C_2$ , and  $C_3$  are material parameters (dependent on  $\eta$ ).

For isotropic material symmetry, (5.126) with  $\boldsymbol{\epsilon}$  from (5.120), yields

$$W = \frac{1}{4} \left\{ \left( \frac{\lambda}{2} + \mu \right) \left[ (\hat{\beta}^2 - 2\hat{\beta})^2 + (a^2 - 2a)^2 \right] + \lambda(\hat{\beta}^2 - 2\hat{\beta})(a^2 - 2a) \right\} \quad (5.128)$$

and

$$\begin{aligned} \mathbf{S}\mathbf{e}_3 &= \lambda(\text{tr } \boldsymbol{\epsilon})\mathbf{e}_3 + 2\mu\boldsymbol{\epsilon}\mathbf{e}_3 \\ &= \frac{1}{2} \left\{ \lambda(\hat{\beta}^2 - 2\hat{\beta}) + (\lambda + 2\mu)(a^2 - 2a) \right\} \mathbf{e}_3. \end{aligned} \quad (5.129)$$

Substitute (5.128) and (5.129) in (5.125) to obtain

$$\left\{ \left( \frac{\lambda}{2} + \mu \right) [\alpha^2 + (a^2 - 2a)^2] + \lambda\alpha(a^2 - 2a) \right\} = a(a-1)\{\lambda\alpha + (\lambda + 2\mu)(a^2 - 2a)\}, \quad (5.130)$$

where  $\alpha = (\hat{\beta}^2 - 2\hat{\beta})$ . Equation (5.130) is quadratic in  $\alpha$ , with all other parameters known.

We can therefore solve (5.130) to obtain  $\alpha$  and thus  $\hat{\beta}$ . The shock speed can be then calculated from (5.124) and (5.129).

For cubic material symmetry, we instead obtain from (5.127) and (5.120)

$$W = \frac{1}{4} \left\{ \frac{C_1}{2} [(\hat{\beta}^2 - 2\hat{\beta})^2 + (a^2 - 2a)^2] + (C_1 + C_2)(\hat{\beta}^2 - 2\hat{\beta})(a^2 - 2a) \right\} \quad (5.131)$$

and

$$\mathbf{S}\mathbf{e}_3 = \frac{1}{2} \left\{ (C_1 + C_2)(\hat{\beta}^2 - 2\hat{\beta}) + C_1(a^2 - 2a) \right\} \mathbf{e}_3. \quad (5.132)$$

Substitute (5.131) and (5.132) in (5.125) to obtain

$$\left\{ \frac{C_1}{2} [\alpha^2 + (a^2 - 2a)^2] + (C_1 + C_2)\alpha(a^2 - 2a) \right\} = a(a-1)\{(C_1 + C_2)\alpha + C_1(a^2 - 2a)\}, \quad (5.133)$$

where  $\alpha = (\hat{\beta}^2 - 2\hat{\beta})$ . Equation (5.133) is quadratic in  $\alpha$ , with all other parameters known.

We can therefore solve (5.133) to obtain  $\alpha$  and thus  $\hat{\beta}$ . The shock speed can be subsequently calculated from (5.124) and (5.132).

**Case (ii)** Consider now, the dislocation wall of type (ii) in figure 5.1. The corresponding surface dislocation density is of the form

$$\boldsymbol{\beta}_r^T = \beta_1 \mathbf{e}_2 \otimes \mathbf{e}_1 + \beta_2 \mathbf{e}_3 \otimes \mathbf{e}_1, \quad (5.134)$$

where  $\{\beta_1, \beta_2\} \in \mathbb{R}$ . Use (5.115) to get

$$\mathbf{K}^{-1} = \mathbf{1} + \beta_1 \mathbf{e}_2 \otimes \mathbf{e}_2 + \beta_2 \mathbf{e}_3 \otimes \mathbf{e}_2, \quad (5.135)$$

whose inverse can be obtained as

$$\mathbf{K} = \mathbf{1} + \hat{\beta}_1 \mathbf{e}_2 \otimes \mathbf{e}_2 + \hat{\beta}_2 \mathbf{e}_3 \otimes \mathbf{e}_2, \quad (5.136)$$

where  $\hat{\beta}_1 = -\frac{\beta_1}{1+\beta_1}$  and  $\hat{\beta}_2 = -\frac{\beta_2}{1+\beta_1}$  (assume  $\beta_1 \neq -1$ ). Further, use relations (5.110) and (5.136) in  $\mathbf{H} = \mathbf{F}\mathbf{K}$  to get

$$\mathbf{H} = \mathbf{1} + \hat{\beta}_1 \mathbf{e}_2 \otimes \mathbf{e}_2 + (1-a)\hat{\beta}_2 \mathbf{e}_3 \otimes \mathbf{e}_2 - a\mathbf{e}_3 \otimes \mathbf{e}_3 \quad (5.137)$$

and similarly use (5.122) and (5.135) in  $\mathbf{H}^{-1} = \mathbf{K}^{-1}\mathbf{F}^{-1}$  to get

$$\mathbf{H}^{-1} = \mathbf{1} + \beta_1 \mathbf{e}_2 \otimes \mathbf{e}_2 + \beta_2 \mathbf{e}_3 \otimes \mathbf{e}_2 + \frac{a}{1-a} \mathbf{e}_3 \otimes \mathbf{e}_3. \quad (5.138)$$

The elastic strain tensor, defined in (5.114), can be evaluated using (5.137) as

$$\boldsymbol{\epsilon} = \frac{1}{2} \{ \gamma \mathbf{e}_2 \otimes \mathbf{e}_2 + \sigma (\mathbf{e}_2 \otimes \mathbf{e}_3 + \mathbf{e}_3 \otimes \mathbf{e}_2) + (a^2 - 2a) \mathbf{e}_3 \otimes \mathbf{e}_3 \}, \quad (5.139)$$

and therefore  $\text{tr } \boldsymbol{\epsilon} = \frac{1}{2}(\gamma + a^2 - 2a)$ , where

$$\gamma = \hat{\beta}_1^2 + 2\hat{\beta}_1 + (1-a)^2 \hat{\beta}_2^2, \quad \text{and } \sigma = (1-a)^2 \hat{\beta}_2. \quad (5.140)$$

Before writing the Hugoniot relations for the case at hand, we make note of the following relations,

$$\mathbf{K}^T \mathbf{e}_3 = \hat{\beta}_2 \mathbf{e}_2 + \mathbf{e}_3, \quad \mathbf{H}^T \mathbf{e}_3 = (1-a)(\hat{\beta}_2 \mathbf{e}_2 + \mathbf{e}_3), \quad \text{and } \mathbf{H}^{-1} \mathbf{e}_3 = \frac{1}{1-a} \mathbf{e}_3, \quad (5.141)$$

which follow from (5.136), (5.137), and (5.138), respectively. Using these, Hugoniot relations (5.112) reduce to

$$\hat{\beta}_2 \mathbf{S} \mathbf{e}_2 + \mathbf{S} \mathbf{e}_3 = -(1 + \hat{\beta}_1) U^2 \rho_\kappa \frac{a}{1-a} \mathbf{e}_3 \quad (5.142)$$

and

$$W = \frac{a(a-1)}{2} (\hat{\beta}_2 \mathbf{S} \mathbf{e}_2 + \mathbf{S} \mathbf{e}_3) \cdot (\hat{\beta}_2 \mathbf{e}_2 + \mathbf{e}_3). \quad (5.143)$$

For isotropic symmetry, stress  $\mathbf{S}$  is constitutively given by (5.126)<sub>2</sub>. Use elastic strain from (5.139) to obtain from (5.126)<sub>2</sub>

$$\mathbf{S}\mathbf{e}_2 = \left\{ \frac{\lambda}{2}(\gamma + a^2 - 2a) + \mu\gamma \right\} \mathbf{e}_2 + \mu\sigma\mathbf{e}_3 \quad \text{and} \quad (5.144)$$

$$\mathbf{S}\mathbf{e}_3 = \left\{ \left( \frac{\lambda}{2} + \mu \right) (a^2 - 2a) + \frac{\lambda}{2}\gamma \right\} \mathbf{e}_3 + \mu\sigma\mathbf{e}_2. \quad (5.145)$$

Taking a dot product of (5.142), with  $\mathbf{e}_2$  and  $\mathbf{e}_3$ , and using equations (5.144) and (5.145), we get

$$\hat{\beta}_2 \left\{ \frac{\lambda}{2}(\gamma + a^2 - 2a) + \mu\gamma \right\} + \mu\sigma = 0 \quad \text{and} \quad (5.146)$$

$$\hat{\beta}_2\mu\sigma + \left\{ \left( \frac{\lambda}{2} + \mu \right) (a^2 - 2a) + \frac{\lambda}{2}\gamma \right\} = -(1 + \hat{\beta}_1)U^2\rho_\kappa \frac{a}{1-a}, \quad (5.147)$$

respectively. Recalling from (5.140)<sub>2</sub> that  $\sigma = (1-a)^2\hat{\beta}_2$ , equation (5.146), for  $\hat{\beta}_2 \neq 0$ , yields

$$\left\{ \frac{\lambda}{2}(\gamma + a^2 - 2a) + \mu\gamma \right\} + \mu(1-a)^2 = 0, \quad (5.148)$$

which, for  $\lambda + 2\mu \neq 0$ , can be rearranged to get an expression for  $\gamma$ :

$$\gamma = (2a - a^2) - \frac{2\mu}{\lambda + 2\mu}. \quad (5.149)$$

On the other hand, the strain energy, as defined in (5.126)<sub>1</sub>, is now of the form

$$W = \frac{\lambda}{8}(\gamma + a^2 - 2a)^2 + \frac{\mu}{4} \{ \gamma^2 + (a^2 - 2a)^2 + 2\sigma^2 \}, \quad (5.150)$$

where we have used elastic strains from (5.139). Substitute this expression for the strain energy in the left side of Hugoniot relation (5.143), and use (5.144) and (5.145) in the right side. We obtain

$$\frac{\lambda}{8}(\gamma + a^2 - 2a)^2 + \frac{\mu}{4} \{ \gamma^2 + (a^2 - 2a)^2 + 2\sigma^2 \} = \frac{a(a-1)}{2} \left\{ \mu(1-a)^2\hat{\beta}_2^2 - \mu(1+\gamma) \right\}, \quad (5.151)$$

where (5.148) has also been used to simplify the left hand side of the equation. Equation (5.151) can be solved for  $\hat{\beta}_2$ , which can be then substituted into (5.140)<sub>1</sub> to obtain  $\hat{\beta}_1$  ( $\gamma$  has been already obtained in (5.149)). Finally, the shock speed can be calculated from equation (5.147).

For cubic symmetry, the strain energy and the stress are given in (5.127). Substituting the elastic strain from (5.139) into them, we can obtain

$$\begin{aligned} W &= \frac{C_1}{8}(\gamma + a^2 - 2a)^2 + \frac{C_2}{4}\gamma(a^2 - 2a) + \frac{C_3}{4}\sigma^2, \\ \mathbf{S}\mathbf{e}_2 &= \frac{C_1}{2}(\gamma + a^2 - 2a)\mathbf{e}_2 + \frac{C_2}{2}(a^2 - 2a)\mathbf{e}_2 + \frac{C_3}{2}\sigma\mathbf{e}_3, \quad \text{and} \\ \mathbf{S}\mathbf{e}_3 &= \frac{C_1}{2}(\gamma + a^2 - 2a)\mathbf{e}_3 + \frac{C_2}{2}\gamma\mathbf{e}_3 + \frac{C_3}{2}\sigma\mathbf{e}_2. \end{aligned} \quad (5.152)$$

Taking a dot product of Hugoniot relation (5.142), with  $\mathbf{e}_2$  and  $\mathbf{e}_3$ , and using equations (5.152)<sub>1,2</sub>, we get

$$\hat{\beta}_2 \frac{C_1}{2}\gamma + \hat{\beta}_2 \frac{(C_1 + C_2)}{2}(a^2 - 2a) + \frac{C_3}{2}\sigma = 0 \quad \text{and} \quad (5.153)$$

$$\hat{\beta}_2 \frac{C_3}{2}\sigma + \frac{C_1}{2}(a^2 - 2a) + \frac{(C_1 + C_2)}{2}\gamma = -(1 + \hat{\beta}_1)U^2\rho_\kappa \frac{a}{1 - a}, \quad (5.154)$$

respectively. Using (5.140)<sub>2</sub> and  $\hat{\beta}_2 \neq 0$ , we can obtain the following expression for  $\gamma$  from (5.153):

$$\gamma = -\frac{1}{C_1} \{ (C_1 + C_2 + C_3)(a^2 - 2a) + C_3 \}. \quad (5.155)$$

On the other hand, Hugoniot relation (5.143), using (5.152), yields

$$\frac{C_1}{2}(\gamma + a^2 - 2a)^2 + C_2\gamma(a^2 - 2a) + C_3\sigma^2 = a(a - 1) \left\{ C_3\hat{\beta}_2^2(1 - a)^2 + C_1(\gamma + a^2 - 2a) + C_2\gamma \right\}. \quad (5.156)$$

Noting (5.140)<sub>2</sub>, equation (5.156) can be solved for  $\hat{\beta}_2$ . Consequently, obtain  $\hat{\beta}_1$  and  $U$  from equations (5.140)<sub>1</sub> and (5.154), respectively.

Finally, note that to evaluate the change in bulk dislocation density in the wake of such dislocation walls, equation (5.50) can be used, which also requires us to know the plastic evolution in the bulk.

### 5.3 Acceleration waves

An acceleration wave is defined as a moving singular surface (i.e.  $U \neq 0$ ) across which the thermodynamic state variables remain continuous, but their derivatives might be discontinuous. In particular, it is necessary for  $\nabla \mathbf{F}$  and thus for  $\dot{\mathbf{v}}$ , to be discontinuous across the singular surface. The name acceleration wave derives from the fact that acceleration is necessarily discontinuous across the wave surface [171, 34]. In the following we discuss the occurrence of such waves in an elastic-plastic medium. Notable earlier work on acceleration waves in elastic-plastic medium can be found in the references [73, 63, 114, 7, 165, 107]. Out of these, only [7] and [107] consider the possibility of finite strains, but use an additive decomposition of the strain.

**Jump conditions** The following two identities will be, in particular very useful for our discussion below: Let  $\mathbf{A}$  be a vector or tensor field defined on  $\kappa_r \times t_1, t_2$ , such that  $\mathbf{A}$  is piecewise continuously differentiable across  $S_t$ . Then

$$[[\nabla \mathbf{A}]] = \mathbf{B} \otimes \mathbf{N} + \nabla^S [[\mathbf{A}]], \quad \text{and} \quad (5.157)$$

$$[[\dot{\mathbf{A}}]] = -U [[\nabla \mathbf{A}]] \mathbf{N} - [[\mathbf{A}]]', \quad (5.158)$$

where  $\mathbf{B}$  is arbitrary. These two relations are generalized from the compatibility conditions (2.69) and (2.72), and their proofs follow those of these conditions.

For an acceleration wave, the following conditions hold

$$[[\mathbf{F}]] = \mathbf{0}, \quad [[\mathbf{v}]] = \mathbf{0}, \quad [[\mathbf{H}]] = \mathbf{0}, \quad \text{and} \quad [[\eta]] = 0. \quad (5.159)$$

Use (5.159)<sub>1</sub> and (5.157) to obtain

$$[[\nabla\mathbf{F}]] = \mathbf{Q} \otimes \mathbf{N} \quad (5.160)$$

for some arbitrary  $\mathbf{Q} \in Lin$ . Since  $F_{ij,k} = \chi_{i,jk}$ , therefore  $F_{ij,k}$  is symmetric with respect to indices  $j$  and  $k$ . Thus, there exists a vector, say  $\mathbf{a} \in \mathcal{V}$ , such that  $\mathbf{Q} = \mathbf{a} \otimes \mathbf{N}$ . Equation (5.160) then becomes

$$[[\nabla\mathbf{F}]] = \mathbf{a} \otimes \mathbf{N} \otimes \mathbf{N}. \quad (5.161)$$

The jump in the time derivative of  $\mathbf{F}$  can then be obtained using (5.159)<sub>1</sub>, (5.158) and (5.161) as

$$[[\dot{\mathbf{F}}]] = -U[[\nabla\mathbf{F}]]\mathbf{N} = -U\mathbf{a} \otimes \mathbf{N}. \quad (5.162)$$

Similarly, we can use (5.159)<sub>2</sub>, (5.158) and (5.162) to obtain the jump in the acceleration field:

$$[[\dot{\mathbf{v}}]] = -U[[\nabla\mathbf{v}]]\mathbf{N} = -U[[\dot{\mathbf{F}}]]\mathbf{N} = U^2\mathbf{a}. \quad (5.163)$$

We will also require jump conditions for (spatial and temporal) derivatives of  $\mathbf{K}^{-1}$  and  $\eta$ . Start by noting that  $[[\mathbf{K}^{-1}]] = \mathbf{0}$ , which follows from (5.159)<sub>1,3</sub> and (3.18). Writing (5.157) and (5.158) for  $\mathbf{K}^{-1}$ , we then have

$$[[\nabla\mathbf{K}^{-1}]] = \mathbf{G} \otimes \mathbf{N}, \quad \text{and} \quad [[\dot{\mathbf{K}}^{-1}]] = -U\mathbf{G}, \quad (5.164)$$

where  $\mathbf{G} \in Lin$  is arbitrary and  $\dot{\mathbf{K}}^{-1}$  denotes the time derivative of  $\mathbf{K}^{-1}$ . Use  $\dot{\mathbf{K}} = -\mathbf{K}\dot{\mathbf{K}}^{-1}\mathbf{K}$  (which follows from  $\mathbf{K}\mathbf{K}^{-1} = \mathbf{1}$ ) to obtain an expression for  $[[\dot{\mathbf{K}}]]$  as

$$[[\dot{\mathbf{K}}]] = U\mathbf{K}\mathbf{G}\mathbf{K}. \quad (5.165)$$



The jump in the true dislocation density  $\boldsymbol{\alpha}$ , for  $\llbracket \mathbf{K}^{-1} \rrbracket = \mathbf{0}$ , follows from (5.69) and (5.70), and takes the form

$$U \llbracket \alpha_{pj} \rrbracket = J_K U K_{pi}^{-1} \llbracket \alpha_{ij}^r \rrbracket = J_K e_{ilk} K_{pi}^{-1} \llbracket \dot{K}_{jl}^{-1} \rrbracket N_k, \quad (5.166)$$

which on substituting from (5.164)<sub>2</sub> becomes

$$\llbracket \alpha_{pj} \rrbracket = J_K e_{ikl} K_{pi}^{-1} G_{jl} N_k. \quad (5.167)$$

Finally, for evaluating jumps in the derivatives of  $\eta$ , write (5.157) and (5.158) for a scalar  $\mathbf{A}$  and obtain

$$\llbracket \nabla \eta \rrbracket = \zeta \mathbf{N}, \quad \text{and} \quad \llbracket \dot{\eta} \rrbracket = -U \zeta, \quad (5.168)$$

where  $\zeta \in \mathbb{R}$  is arbitrary.

**Governing equations** The balance laws for mass and linear momentum, away and on the singular surface, were obtained in equations (2.129), (2.130), (2.143), and (2.144). We rewrite them below:

$$\dot{\rho}_\kappa = 0, \quad \llbracket \rho_\kappa \rrbracket = 0, \quad \text{and} \quad (5.169)$$

$$\rho_\kappa \dot{\mathbf{v}} = \text{Div } \mathbf{P} + \rho_\kappa \mathbf{b}, \quad \llbracket \mathbf{P} \rrbracket \mathbf{N} + U \llbracket \rho_\kappa \mathbf{v} \rrbracket = \mathbf{0}. \quad (5.170)$$

The statements of balance of energy, for adiabatic processes, were obtained in (3.95) and (3.89) and are repeated below:

$$\rho_\kappa \theta \dot{\eta} = J_K^{-1} \mathbf{E}' \cdot \mathbf{K}^{-1} \dot{\mathbf{K}}, \quad \text{and} \quad U \llbracket J_K^{-1} W \rrbracket = U \langle \mathbf{P} \rangle \cdot \llbracket \mathbf{F} \rrbracket, \quad (5.171)$$

where  $\mathbf{E}' = W \mathbf{1} - \mathbf{H}^T W_{\mathbf{H}}$ , outside and on the singular surface, respectively. To these balance laws, restrictions from the second law should also be appended. We have from

(3.96) and (3.97)

$$J_K^{-1} \mathbf{E}' \cdot \mathbf{K}^{-1} \dot{\mathbf{K}} \geq 0, \quad \text{and} \quad -U \rho_\kappa \llbracket \eta \rrbracket \geq 0. \quad (5.172)$$

Finally, we make the following constitutive assumptions (cf. (3.91))

$$W = W(\mathbf{H}, \eta), \quad \mathbf{P} = J_K^{-1} W_{\mathbf{H}} \mathbf{K}^T, \quad \text{and} \quad \rho_\kappa \theta = J_K^{-1} W_\eta. \quad (5.173)$$

Noting the jump conditions (5.159), it immediately follows from the above constitutive hypothesis that

$$\llbracket W \rrbracket = 0, \quad \llbracket \mathbf{P} \rrbracket = \mathbf{0}, \quad \text{and} \quad \llbracket \theta \rrbracket = 0 \quad (5.174)$$

Substituting these and (5.159) into (5.170)<sub>2</sub>, (5.171)<sub>2</sub>, and (5.172)<sub>2</sub>, it turns out that the jump conditions for balance of mass and momentum, and the dissipation inequality at the surface, all are trivially satisfied for acceleration waves. As we will see below, this simplifies our problem considerably. Moreover, note that there is no inherent dissipation involved with the propagation of acceleration waves. The only source for dissipation in an adiabatic process is plastic evolution in the neighborhood of the propagating wave (given by (5.172)<sub>1</sub>). There is no dissipation *at* the singular surface. For an elastic acceleration wave (Subsection 5.3.1 below), therefore, there is no dissipation and the propagation of an acceleration wave is a reversible process. Moreover, the condition (5.159)<sub>3</sub> excludes the possibility of surface dislocations at all acceleration waves (cf. (5.13)).

Our problem here, is to obtain the wave speed and the first order derivatives of state variables behind the wave, for known values of these derivatives ahead of the wave. Referring to equations (5.161)–(5.168), we are therefore interested to solve for  $\mathbf{a}$ ,  $\mathbf{G}$ ,  $\zeta$ , and  $U$ . These in general are fourteen unknowns. We would now obtain the set of governing equations for obtaining these unknowns. Start by writing relations (5.170)<sub>1</sub> and (5.171)<sub>1</sub>

for both sides of the surface, and evaluating their difference. For  $[[\mathbf{b}]] = \mathbf{0}$ , equation (5.170)<sub>1</sub> on using (5.169)<sub>2</sub>, gives us

$$[[\text{Div } \mathbf{P}]] = \rho_\kappa [[\dot{\mathbf{v}}]], \quad (5.175)$$

and equation (5.171)<sub>1</sub> on using (5.174), yields

$$\rho_\kappa \theta [[\dot{\eta}]] = J_K^{-1} \mathbf{E}' \cdot \mathbf{K}^{-1} [[\dot{\mathbf{K}}]]. \quad (5.176)$$

Recall jump conditions (5.165) and (5.168)<sub>2</sub>, and use them to rewrite the relation (5.176) as

$$\rho_\kappa \theta \zeta = -J_K^{-1} \mathbf{E}' \cdot \mathbf{G}\mathbf{K}. \quad (5.177)$$

To express (5.175) in terms of our unknowns, first note the condition (5.174)<sub>2</sub>, and obtain the jump in the gradient of  $\mathbf{P}$  using (5.157)

$$[[\nabla \mathbf{P}]] = \mathbf{Z} \otimes \mathbf{N}, \quad (5.178)$$

where  $\mathbf{Z} \in \text{Lin}$  is arbitrary. Equation (5.178) implies

$$[[\text{Div } \mathbf{P}]] = \mathbf{Z}\mathbf{N}. \quad (5.179)$$

On the other hand, using (5.158) we have

$$[[\dot{\mathbf{P}}]] = -U\mathbf{Z}. \quad (5.180)$$

The tensor  $\mathbf{Z}$  can be eliminated between equations (5.179) and (5.180) to get

$$[[\dot{\mathbf{P}}]]\mathbf{N} = -U[[\text{Div } \mathbf{P}]]. \quad (5.181)$$

Substituting this and (5.163) into (5.175) we obtain

$$[[\dot{\mathbf{P}}]]\mathbf{N} = -\rho_\kappa U^3 \mathbf{a}. \quad (5.182)$$

We can now use the constitutive hypothesis (5.173)<sub>2</sub> and the chain rule to write

$$\dot{\mathbf{P}} = (\text{tr } \mathbf{K}\dot{\mathbf{K}}^{-1})\mathbf{P} + J_K^{-1}W_{\mathbf{H}\mathbf{H}}[\dot{\mathbf{H}}]\mathbf{K}^T + J_K^{-1}\dot{\eta}W_{\eta\mathbf{H}}\mathbf{K}^T + J_K^{-1}W_{\mathbf{H}}\dot{\mathbf{K}}^T. \quad (5.183)$$

Use  $\dot{\mathbf{H}} = \dot{\mathbf{F}}\mathbf{K} + \mathbf{F}\dot{\mathbf{K}}$  in (5.183) to rewrite it as

$$\dot{\mathbf{P}} = (\text{tr } \mathbf{K}\dot{\mathbf{K}}^{-1})\mathbf{P} + J_K^{-1}W_{\mathbf{H}\mathbf{H}}[\dot{\mathbf{F}}\mathbf{K}]\mathbf{K}^T + J_K^{-1}W_{\mathbf{H}\mathbf{H}}[\mathbf{F}\dot{\mathbf{K}}]\mathbf{K}^T + J_K^{-1}\dot{\eta}W_{\eta\mathbf{H}}\mathbf{K}^T + \mathbf{P} \left( \dot{\mathbf{K}}\mathbf{K}^{-1} \right)^T. \quad (5.184)$$

This can be used to calculate  $\llbracket \dot{\mathbf{P}} \rrbracket$  in terms of the unknowns. To this effect, obtain using (5.162), (5.164)<sub>2</sub>, (5.165), and (5.168)<sub>2</sub>

$$\frac{-J_K}{U} \llbracket \dot{\mathbf{P}} \rrbracket = J_K(\text{tr } \mathbf{K}\mathbf{G})\mathbf{P} + W_{\mathbf{H}\mathbf{H}}[\mathbf{a} \otimes \mathbf{K}^T \mathbf{N}]\mathbf{K}^T - W_{\mathbf{H}\mathbf{H}}[\mathbf{H}\mathbf{G}\mathbf{K}]\mathbf{K}^T + \zeta W_{\eta\mathbf{H}}\mathbf{K}^T - J_K \mathbf{P} (\mathbf{K}\mathbf{G})^T, \quad (5.185)$$

where we have also used conditions (5.159) and (5.174). Define

$$\tilde{\mathbf{N}} = \mathbf{K}^T \mathbf{N}. \quad (5.186)$$

Recall Nanson's formula,  $\mathbf{N}dA = \mathbf{K}^* \mathbf{N}^i dA^i$ , which relates the unit normal  $\mathbf{N}^i$  associated with the (image of) singular surface in the intermediate configuration<sup>6</sup> to the unit normal  $\mathbf{N}$  in the reference configuration. Here  $dA^i$  and  $dA$  are the infinitesimal areas of the surface in the intermediate and the reference configuration, respectively. Let  $j = \frac{dA}{dA^i}$  be the ratio of these areas. Comparing the stated Nanson's formula with (5.186), we can then conclude that

$$\tilde{\mathbf{N}} = J_K \frac{dA^i}{dA} \mathbf{N}^i, \quad \text{with } |\tilde{\mathbf{N}}| = J_K j^{-1} \equiv j, \text{ say.} \quad (5.187)$$

---

<sup>6</sup>Since  $\llbracket \mathbf{K} \rrbracket = \mathbf{0}$ , the tangent plane  $T_{S_t(\mathbf{X})}$  at some point  $\mathbf{X}$  on the singular surface  $S_t$  is mapped into an unique tangent plane at the point  $p = \kappa_i(\kappa_r^{-1}(\mathbf{X}))$  in the relaxed configuration (cf. Remark 5.1.3). As a result the normal  $\mathbf{N}^i$  is unique.

Therefore  $\tilde{\mathbf{N}} = j\mathbf{N}^i$ , with  $|\mathbf{N}^i| = 1$ . Operate both sides of the equality (5.185) on normal  $\mathbf{N}$  and use the definition (5.186) to obtain

$$\frac{-J_K}{U} \llbracket \dot{\mathbf{P}} \rrbracket \mathbf{N} = (\text{tr } \mathbf{K}\mathbf{G})W_{\mathbf{H}}\tilde{\mathbf{N}} + W_{\mathbf{H}\mathbf{H}}[\mathbf{a} \otimes \tilde{\mathbf{N}}]\tilde{\mathbf{N}} - W_{\mathbf{H}\mathbf{H}}[\mathbf{H}\mathbf{G}\mathbf{K}]\tilde{\mathbf{N}} + \zeta W_{\eta\mathbf{H}}\tilde{\mathbf{N}} - J_K \mathbf{P}\mathbf{G}^T \tilde{\mathbf{N}}, \quad (5.188)$$

where (5.173)<sub>2</sub> has been used in the first term on the right hand side. Substitute first the expression for  $\zeta$  from (5.177) into (5.188) and then the resulting expression for  $\llbracket \dot{\mathbf{P}} \rrbracket \mathbf{N}$  into (5.182). Obtain

$$j^{-1}\mathbb{A}[\mathbf{G}] + \mathbf{Q}\mathbf{a} = \rho_r \tilde{U}^2 \mathbf{a} \quad (5.189)$$

or in the indicial notation (with respect to Cartesian coordinate system)

$$j^{-1}\mathbb{A}_{ijk}G_{jk} + Q_{ij}a_j = \rho_r \tilde{U}^2 a_i, \quad (5.190)$$

where  $\rho_r = J_K \rho_\kappa$  is the mass density per unit volume of the relaxed configuration and  $\tilde{U} = j^{-1}U$ . The third order tensor  $\mathbb{A}$  and the second order tensor  $\mathbf{Q}$  are given by

$$\begin{aligned} \mathbb{A}_{ijk} &= (W_{\mathbf{H}})_{im}N_m^i K_{jk} - (W_{\mathbf{H}\mathbf{H}})_{impq}N_m^i H_{pj}K_{kq} \\ &\quad - \frac{1}{\rho_r \theta} (W_{\eta\mathbf{H}})_{im}N_m^i E'_{jq}K_{kq} + J_K P_{ik}N_j^i, \text{ and} \end{aligned} \quad (5.191)$$

$$Q_{ij} = (W_{\mathbf{H}\mathbf{H}})_{ikjm}N_k^i N_m^j. \quad (5.192)$$

The tensor  $\mathbf{Q}$  is sometimes known as the *elastic acoustic tensor* in the theory of elastic waves.

In addition to (5.177) and (5.189), we can obtain another governing equation from the flow rule which dictates the plastic flow in the neighborhood of the wave. A general flow rule of the following form can be assumed: (cf. (3.130))

$$\dot{\mathbf{K}}^{-1}\mathbf{K} = \mathcal{H}(\mathbf{C}_H, \dot{\mathbf{C}}_H, \boldsymbol{\alpha}, \eta, \dot{\eta}, \nabla\eta\mathbf{K}). \quad (5.193)$$

Note that, in comparison with (3.130), we have used  $\eta$  instead of  $\theta$  (since we are assuming adiabatic response). If plasticity evolves on both sides of the wave surface, then (5.193) can be written for the sides. Subtracting the resulting expressions and using (5.164)<sub>2</sub> we get

$$-UG\mathbf{K} = \llbracket \mathcal{H} \rrbracket. \quad (5.194)$$

In general,  $\llbracket \mathcal{H} \rrbracket$  can be a highly nonlinear function of  $\mathbf{a}$ ,  $\mathbf{G}$  and  $\zeta$ . Any further analytical investigation will require a specific form of  $\mathcal{H}$ , which would then determine the complexity of the problem. This is done in Subsection 5.3.2 below, where we assume a rate independent response and an associated flow rule.

If, however, plastic flow is only restricted to behind the wave, which is the case of a loading plastic wave, then (5.194) reduces to

$$UG\mathbf{K} = \mathcal{H}^- \quad (5.195)$$

since  $\mathcal{H}^+ = \mathbf{0}$ . Also, using  $\dot{\mathbf{K}}^{-1+} = \mathbf{0}$  in (5.164)<sub>2</sub> implies that  $\dot{\mathbf{K}}^{-1-} = U\mathbf{G}$ . On the other hand, for an unloading plastic wave, plasticity evolves only ahead of the wave, i.e.  $\dot{\mathbf{K}}^{-1+} \neq \mathbf{0}$  but  $\dot{\mathbf{K}}^{-1-} = \mathbf{0}$ . In this case, assuming  $\dot{\mathbf{K}}^{-1+}$  to be known,  $\mathbf{G}$  follows directly from (5.164)<sub>2</sub> as  $UG = -\dot{\mathbf{K}}^{-1+}$ .

### 5.3.1 Elastic acceleration wave

An elastic acceleration wave is defined as the acceleration wave with no plastic evolution in its neighborhood. This implies  $\dot{\mathbf{K}}^\pm = \mathbf{0}$  and consequently  $\mathbf{G} = \mathbf{0}$ . As is evident from (5.167), there can be no jump in the dislocation density  $\alpha$  across such waves. Moreover  $\zeta = 0$ , which follows from (5.177). Therefore our problem is reduced to determining  $\mathbf{a}$  and  $U$ .

For  $\mathbf{G} = \mathbf{0}$ , (5.190) reduces to

$$(Q_{ij} - \rho_r \tilde{U}^2 \delta_{ij}) a_j = 0, \quad (5.196)$$

where  $Q_{ij}$  is given in (5.192). The elastic acoustic tensor  $Q_{ij}$  is symmetric and therefore has three real eigenvalues. The positive eigenvalues will correspond to real wave speeds.

The strain energy is usually given in terms of  $\mathbf{C}_H$  rather than  $\mathbf{H}$ , i.e. we have  $W(\mathbf{H}, \eta) = \hat{W}(\mathbf{C}_H, \eta)$ . It would therefore be useful to express  $W_{\mathbf{H}}$  and  $W_{\mathbf{H}\mathbf{H}}$  in terms of  $\hat{W}_{\mathbf{C}_H}$  and  $\hat{W}_{\mathbf{C}_H \mathbf{C}_H}$ . Use  $\mathbf{C}_H = \mathbf{H}^T \mathbf{H}$  and the chain rule to obtain

$$(W_{\mathbf{H}})_{ik} = 2H_{il} \underset{lk}{Sym}(\hat{W}_{\mathbf{C}_H})_{lk}, \quad (5.197)$$

where  $2\underset{lk}{Sym}(A_{lk}) = A_{lk} + A_{kl}$ , for  $\mathbf{A} \in Lin$ . Differentiate (5.197)<sub>1</sub> with respect to  $\mathbf{H}$  and use the chain rule to get

$$(W_{\mathbf{H}\mathbf{H}})_{ikjm} = 2\delta_{ij} \underset{lk}{Sym}(\hat{W}_{\mathbf{C}_H})_{lk} + 4H_{il} H_{jn} \underset{lk,mn}{Sym}(\hat{W}_{\mathbf{C}_H})_{lkmn}, \quad (5.198)$$

where  $4\underset{lk,mn}{Sym}(\mathcal{B}_{lkmn}) = \mathcal{B}_{lkmn} + \mathcal{B}_{klmn} + \mathcal{B}_{lknm} + \mathcal{B}_{klmn}$  (here  $\mathcal{B}$  is an arbitrary fourth order tensor). Denote

$$\mathbb{C}_{lkmn} = 4\underset{lk,mn}{Sym}(\hat{W}_{\mathbf{C}_H})_{lkmn} \quad (5.199)$$

as the elasticity tensor. Also, recall that  $S_{lk} = 2\underset{lk}{Sym}(\hat{W}_{\mathbf{C}_H})_{lk}$  (cf. (3.101)). Use these to rewrite (5.197) and (5.198) as

$$(W_{\mathbf{H}})_{ik} = H_{il} S_{lk}, \quad \text{and} \quad (W_{\mathbf{H}\mathbf{H}})_{ikjm} = \delta_{ij} S_{lk} + H_{il} H_{jn} \mathbb{C}_{lkmn}, \quad (5.200)$$

respectively.

For small elastic strain  $\epsilon$ ,  $\mathbf{H} = \mathbf{R} + O(|\epsilon|)$ ,  $\mathbf{S} = O(|\epsilon|)$ , and  $\mathbb{C} = O(1)$ , where  $\mathbf{R} \in Orth^+$  is the rotation in the polar decomposition of  $\mathbf{H}$ . Therefore for small elastic

strain

$$(W_{\mathbf{H}})_{ik} \approx R_{il}S_{lk}, \quad \text{and} \quad (W_{\mathbf{HH}})_{ikjm} \approx R_{il}R_{jn}\mathbb{C}_{lkmn}. \quad (5.201)$$

In the following, we will use (5.201)<sub>2</sub>, (5.192), and (5.196) to obtain explicit representations for the acoustic tensor for the case of isotropic and cubic symmetry. We obtain the classical results for wave speeds in an isotropic medium, which are independent of the direction of wave propagation (i.e. of  $\mathbf{N}^i$ ). However, for the cubic case, the wave speeds depend on  $\mathbf{N}^i$  and the situation is far more complicated than the isotropic case.<sup>7</sup> The strain energy for these two crystal classes are given in (5.126)<sub>1</sub> and (5.127)<sub>1</sub>. We can use these and the definition of elastic strain (5.120) in (5.199), to obtain  $\mathbb{C}$  for isotropic and cubic symmetry groups as

$$\mathbb{C}_{lkmn} = \lambda\delta_{lk}\delta_{mn} + \mu(\delta_{lm}\delta_{kn} + \delta_{ln}\delta_{km}), \quad \text{and} \quad (5.202)$$

$$\mathbb{C}_{lkmn} = C_1\delta_{lk}\delta_{mn} + C_2\mathbb{H}_{lkmn} + \frac{C_3}{2}\mathbb{K}_{lkmn}, \quad (5.203)$$

respectively, where  $\mathbb{H}$  and  $\mathbb{K}$  are constant fourth order tensors defined by

$$\begin{aligned} \mathbb{H} &= (\mathbf{e}_2 \otimes \mathbf{e}_2 + \mathbf{e}_3 \otimes \mathbf{e}_3)\mathbf{e}_1 \otimes \mathbf{e}_1 + (\mathbf{e}_1 \otimes \mathbf{e}_1 + \mathbf{e}_3 \otimes \mathbf{e}_3)\mathbf{e}_2 \otimes \mathbf{e}_2 \\ &+ (\mathbf{e}_1 \otimes \mathbf{e}_1 + \mathbf{e}_2 \otimes \mathbf{e}_2)\mathbf{e}_3 \otimes \mathbf{e}_3, \quad \text{and} \end{aligned} \quad (5.204)$$

$$\begin{aligned} \mathbb{K} &= (\mathbf{e}_1 \otimes \mathbf{e}_2 + \mathbf{e}_2 \otimes \mathbf{e}_1)(\mathbf{e}_1 \otimes \mathbf{e}_2 + \mathbf{e}_2 \otimes \mathbf{e}_1) + (\mathbf{e}_1 \otimes \mathbf{e}_3 + \mathbf{e}_3 \otimes \mathbf{e}_1)(\mathbf{e}_1 \otimes \mathbf{e}_3 + \mathbf{e}_3 \otimes \mathbf{e}_1) \\ &+ (\mathbf{e}_3 \otimes \mathbf{e}_2 + \mathbf{e}_2 \otimes \mathbf{e}_3)(\mathbf{e}_3 \otimes \mathbf{e}_2 + \mathbf{e}_2 \otimes \mathbf{e}_3), \end{aligned} \quad (5.205)$$

where  $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$  is a fixed orthonormal basis in  $\mathcal{E}$ . Substitute (5.202) into (5.201)<sub>2</sub> and

---

<sup>7</sup>Fundamental studies in the subject of elastic waves in anisotropic solids were conducted by Fedorov [50] and Musgrave [121]. Owing to much complexity of the problem of obtaining any exact solutions, most of the recent work on this subject concentrates on obtaining bounds for wave speeds [15].



use the result in (5.192) to obtain the elastic acoustic tensor for isotropic symmetry

$$\mathbf{Q} = (\lambda + \mu)\check{\mathbf{N}} \otimes \check{\mathbf{N}} + \mu\mathbf{1}, \quad (5.206)$$

where  $\check{\mathbf{N}} = \mathbf{R}\mathbf{N}^i$  is a unit vector (since  $|\check{\mathbf{N}}|^2 = |\mathbf{R}\mathbf{N}^i|^2 = 1$ ). One eigenvalue of  $Q_{ij}$  is  $\lambda + 2\mu$  corresponding to eigenvector  $\check{\mathbf{N}}$ . The other eigen value is  $\mu$  with a multiplicity of two, and with eigenvector lying in the plane orthogonal to  $\check{\mathbf{N}}$ . The wave speeds follow from (5.196):

$$\tilde{U}_1^e = \sqrt{\frac{\lambda + 2\mu}{\rho_r}}, \quad \text{and} \quad \tilde{U}_2^e = \sqrt{\frac{\mu}{\rho_r}}. \quad (5.207)$$

Both of these speeds are real, since  $\lambda + 2\mu > 0$  and  $\mu > 0$  (cf. (3.124)).

On the other hand, the situation is not so simple for cubic symmetry. To evaluate the relevant acoustic tensor, start by obtaining the following identities (using (5.204) and (5.205)),

$$\mathbf{N}^i \cdot \mathbb{H} \cdot \mathbf{N}^i = \mathbf{N}^i \otimes \mathbf{N}^i - \sum_{a=1}^3 N_a^i \mathbf{e}_a \otimes \mathbf{e}_a, \quad \text{and} \quad (5.208)$$

$$\mathbf{N}^i \cdot \mathbb{K} \cdot \mathbf{N}^i = \mathbf{1} + \mathbf{N}^i \otimes \mathbf{N}^i - 2 \sum_{a=1}^3 N_a^i \mathbf{e}_a \otimes \mathbf{e}_a, \quad (5.209)$$

where  $N_a^i = \mathbf{N}^i \cdot \mathbf{e}_a$ . Substitute these in (5.203) to get

$$\mathbf{N}^i \cdot \mathbb{C} \cdot \mathbf{N}^i = \frac{C_3}{2} \mathbf{1} + (C_1 + C_2 + \frac{C_3}{2}) \mathbf{N}^i \otimes \mathbf{N}^i - (C_2 + C_3) \sum_{a=1}^3 N_a^i \mathbf{e}_a \otimes \mathbf{e}_a. \quad (5.210)$$

The acoustic tensor  $\mathbf{Q}$  then follows on using (5.210) and (5.201)<sub>2</sub> in (5.192). We obtain (see also [121])

$$\mathbf{Q} = \frac{C_3}{2} \mathbf{1} + (C_1 + C_2 + \frac{C_3}{2}) \check{\mathbf{N}}^i \otimes \check{\mathbf{N}}^i - (C_2 + C_3) \sum_{a=1}^3 N_a^i \check{\mathbf{e}}_a \otimes \check{\mathbf{e}}_a, \quad (5.211)$$

where  $\check{\mathbf{N}} = \mathbf{R}\mathbf{N}^i$  and  $\check{\mathbf{e}}_a = \mathbf{R}\mathbf{e}_a$ . It is evident from (5.211), that in general, the eigenvalues of  $\mathbf{Q}$  will be functions of  $\mathbf{N}^i$ , and so will be the eigenvectors.

### 5.3.2 Plastic acceleration wave

For a plastic acceleration wave  $\dot{\mathbf{K}}^\pm \neq \mathbf{0}$ , which implies that  $\mathbf{G} \neq \mathbf{0}$ . Therefore, contrary to an elastic acceleration wave, a plastic acceleration wave is always accompanied by a plastic evolution in the neighboring bulk. Moreover, as implied from (5.167) and (5.177), there will be, in general, a jump in the dislocation density and rate of specific entropy across the wave surface.

The contents of this subsection are divided into two parts. We start by obtaining a necessary and sufficient condition for dislocation density to be continuous across a plastic acceleration wave. According to this condition, the jump in plastic distortion rate is rank one. Next, we restrict our attention to rate independent flow rules and obtain the governing equations for both non-hardening and hardening plastic evolution.

**Consequence of a continuous  $\alpha$**  In our model of plastic flow, a dependence of yield and flow rule on  $\alpha$  is the only source of work hardening (cf. Section 3.7 and Remark 3.8.1). Therefore, the continuity of  $\alpha$  is a sufficient condition for continuous work hardening across the wave. Necessary conditions can of course only be obtained once the specific forms of flow rule and the yield are assumed. It should be noted that in most of the previous work in plastic acceleration waves, hardening parameter has been assumed to be continuous. However, as we shall see below, the assumption of continuous  $\alpha$  restricts the plastic distortion rate to a rank one form, which proves to be too restrictive even for the simplest of flow rules.

For a continuous  $\mathbf{K}$ , the true dislocation density  $\alpha$  is related to the referential dislocation density by (5.166)<sub>1</sub>, from which it is evident that  $[[\alpha]] = \mathbf{0}$  if and only if  $[[\alpha_r]] = \mathbf{0}$ .

The compatibility relation between the jump in  $\alpha_r$  and the jump in plastic distortion rate is given in (5.70). Take the material time derivative of the identity  $\mathbf{K}\mathbf{K}^{-1} = \mathbf{1}$  and use the result in (5.70) to obtain

$$U[\alpha_{ij}^r] = e_{ikl}K_{jm}^{-1}K_{nl}^{-1}[\dot{K}_{mn}]N_k. \quad (5.212)$$

It follows immediately from (5.212) that

$$[\alpha_{ij}^r]N_i = 0, \quad (5.213)$$

$$U[\alpha_{ij}^r]t_{1i} = -K_{jm}^{-1}K_{nl}^{-1}[\dot{K}_{mn}]t_{2l}, \quad \text{and} \quad (5.214)$$

$$U[\alpha_{ij}^r]t_{2i} = K_{jm}^{-1}K_{nl}^{-1}[\dot{K}_{mn}]t_{1l}, \quad (5.215)$$

where  $\{\mathbf{t}_1, \mathbf{t}_2, \mathbf{N}\} \in \mathcal{V}$  form a right handed orthogonal triad at every point on the singular surface  $S_t$ . Let  $\tilde{\mathbf{t}}_1 = \mathbf{K}^{-1}\mathbf{t}_1$  and  $\tilde{\mathbf{t}}_2 = \mathbf{K}^{-1}\mathbf{t}_2$ . The triad of vectors  $\{\tilde{\mathbf{t}}_1, \tilde{\mathbf{t}}_2, \tilde{\mathbf{N}}\} \in T_{\mathcal{M}}$ , where  $\tilde{\mathbf{N}}$  is defined in (5.186), form a basis in the tangent space to the surface in relaxed configuration. This claim can be verified by first noting the following identities

$$\tilde{\mathbf{t}}_a \cdot \tilde{\mathbf{N}} = \mathbf{K}^{-1}\mathbf{t}_a \cdot \mathbf{K}^T\mathbf{N} = \mathbf{t}_a \cdot \mathbf{N} = 0 \quad (5.216)$$

$$\mathbf{K}^{-1}\mathbf{t}_a \cdot \mathbf{K}^T\mathbf{t}_b = \delta_{ab}, \quad (5.217)$$

where  $a, b \in \{1, 2\}$ . Identities (5.216) prove that vectors  $\{\tilde{\mathbf{t}}_1, \tilde{\mathbf{t}}_2\}$  lie in the plane orthogonal to  $\tilde{\mathbf{N}}$ . It remains to be shown that  $\tilde{\mathbf{t}}_1$  and  $\tilde{\mathbf{t}}_2$  are not parallel to each other. Assume that  $\tilde{\mathbf{t}}_1$  and  $\tilde{\mathbf{t}}_2$  are parallel to each other. Use  $\{a, b\} = \{1, 2\}$  and  $\{a, b\} = \{2, 2\}$  in (5.217) to obtain  $\mathbf{K}^{-1}\mathbf{t}_1 \cdot \mathbf{K}^T\mathbf{t}_2 = 0$  and  $\mathbf{K}^{-1}\mathbf{t}_2 \cdot \mathbf{K}^T\mathbf{t}_2 = 1$ , respectively. The first of these imply that  $\mathbf{K}^T\mathbf{t}_2$  is perpendicular to  $\tilde{\mathbf{t}}_1$  and therefore to  $\tilde{\mathbf{t}}_2$ , a fact contrary to the second relation. Therefore,  $\tilde{\mathbf{t}}_1$  and  $\tilde{\mathbf{t}}_2$  are not parallel to each other, and we have proved that  $\{\tilde{\mathbf{t}}_1, \tilde{\mathbf{t}}_2, \tilde{\mathbf{N}}\}$  can form a valid basis in the tangent space to the surface in  $\kappa_i$ .

Equations (5.213)-(5.215) then imply that  $\alpha_r$  is continuous across the wave if and only if the tangential components of the plastic distortion rate are continuous, i.e. when  $[[\dot{\mathbf{K}}]]\tilde{\mathbf{t}}_a = \mathbf{0}$  for  $a \in \{1, 2\}$ . Thus, the jump in  $\dot{\mathbf{K}}$  has the following form:

$$[[\dot{\mathbf{K}}]] = \mathbf{h} \otimes \tilde{\mathbf{N}}, \quad (5.218)$$

where  $\mathbf{h} \in \mathcal{V}$  is arbitrary.

We now consider a simple flow rule and show that a condition of the type can be too restrictive on the nature of stress state. Assume (cf. (4.72))

$$\mathbf{K}^{-1}\dot{\mathbf{K}} = \sigma \mathbf{S}^d, \quad (5.219)$$

where  $\sigma \in \mathbb{R}^+$  is a scalar valued function and  $\mathbf{S}^d$  is the deviatoric part of  $\mathbf{S}$ . Associated flow rules, with isotropic symmetry and von Mises yield criteria, have the same form as (5.219). Eliminating  $\dot{\mathbf{K}}$  between (5.218) and (5.219) we get

$$[[\sigma]]\mathbf{S}^d = \mathbf{K}^{-1}\mathbf{h} \otimes \tilde{\mathbf{N}}. \quad (5.220)$$

This is indeed a severe restriction on the form of  $\mathbf{S}^d$ , and something which does not hold in general.

In conclusion, a continuous dislocation density across the wave might impose unnecessary physical restrictions. Therefore we will, in general, allow for a discontinuous  $\alpha$  in our treatment of plastic acceleration waves.

**Rate independent plastic flow** For a rate independent plastic flow, the flow rule assumed in (5.193) should be insensitive to the time scale. This implies that  $\mathcal{H}$  is homogeneous of degree one in both,  $\dot{\mathbf{C}}_H$  and  $\dot{\eta}$ . The flow rule then takes the form

$$\mathbf{K}^{-1}\dot{\mathbf{K}} = \mathcal{P}(\mathbf{C}_H, \alpha, \eta, \nabla\eta\mathbf{K})[\dot{\mathbf{C}}_H] + \mathbf{M}(\mathbf{C}_H, \alpha, \eta, \nabla\eta\mathbf{K})\dot{\eta}. \quad (5.221)$$

where  $\mathcal{P}$  and  $\mathbf{M}$  are fourth order and second order tensors, respectively. Moreover, the tensor  $\mathcal{P}$  has a minor symmetry with respect to last two indices.<sup>8</sup> Use  $\mathbf{C}_H = \mathbf{H}^T \mathbf{H}$ ,  $\dot{\mathbf{H}} = \dot{\mathbf{F}} \mathbf{K} + \mathbf{F} \dot{\mathbf{K}}$ , and  $\dot{\mathbf{K}} = -\mathbf{K} \dot{\mathbf{K}}^{-1} \mathbf{K}$  to obtain

$$\dot{\mathbf{C}}_H = 2Sym(\mathbf{H}^T \dot{\mathbf{F}} \mathbf{K} - \mathbf{C}_H \dot{\mathbf{K}}^{-1} \mathbf{K}). \quad (5.222)$$

Substituting  $\dot{\mathbf{C}}_H$  and  $\dot{\eta}$  from (5.222) and (5.171)<sub>1</sub>, respectively, into (5.221) yields

$$\dot{\mathbf{K}}^{-1} \mathbf{K} = 2\mathcal{P}[\mathbf{H}^T \dot{\mathbf{F}} \mathbf{K} - \mathbf{C}_H \dot{\mathbf{K}}^{-1} \mathbf{K}] - \frac{1}{\rho_r \theta} (\mathbf{M} \otimes \mathbf{E}') [\dot{\mathbf{K}}^{-1} \mathbf{K}], \quad (5.223)$$

where we have also used the minor symmetry of  $\mathcal{P}$ . We can rearrange (5.223) to get

$$\mathcal{Q}[\dot{\mathbf{K}}^{-1} \mathbf{K}] = \mathcal{R}[\dot{\mathbf{F}}], \quad (5.224)$$

where

$$\mathcal{Q}_{ijkl} = \mathbb{I}_{ijkl} + 2\mathcal{P}_{ijml} C_{mk}^H + \frac{1}{\rho_r \theta} (\mathbf{M} \otimes \mathbf{E}')_{ijkl}, \quad \text{and} \quad (5.225)$$

$$\mathcal{R}_{ijkl} = 2\mathcal{P}_{ijmn} H_{km} K_{ln}. \quad (5.226)$$

But in order to obtain an expression for  $\dot{\mathbf{K}}^{-1} \mathbf{K}$  from (5.224), we would require  $\mathcal{Q}$  to be invertible. As we will see below, this is indeed true in the case of associated flow rules.

Assuming, for now, that  $\mathcal{Q}$  is invertible, (5.224) yields

$$\dot{\mathbf{K}}^{-1} \mathbf{K} = \mathcal{T}[\dot{\mathbf{F}}], \quad \text{where } \mathcal{T} = \mathcal{Q}^{-1} \mathcal{R} \quad (5.227)$$

is a fourth order tensor function of  $\{\mathbf{H}, \mathbf{K}, \boldsymbol{\alpha}, \eta, \nabla \eta \mathbf{K}\}$ , and therefore in general, is not continuous across the wave. Evaluate (5.227) at both sides of the interface, take the difference

---

<sup>8</sup>This symmetry appears due to the symmetric  $\dot{\mathbf{C}}_H$ . For some basic properties of a fourth order tensor, see the paragraph on page 22.

of the resulting equations and use (5.164)<sub>2</sub> to get

$$-U\mathbf{G}\mathbf{K} = \llbracket \mathcal{T}[\dot{\mathbf{F}}] \rrbracket = \llbracket \mathcal{T} \rrbracket [\dot{\mathbf{F}}^+] - U\mathcal{T}^-[\mathbf{a} \otimes \mathbf{N}], \quad (5.228)$$

where the second equality results on using relations (2.46) and (5.162). It should be noted here that by virtue of conditions (5.167), (5.168), and (5.177), both  $\llbracket \mathcal{T} \rrbracket$  and  $\mathcal{T}^-$  would be functions of  $\mathbf{G}$ . This dependence can be ascertained only after specific forms of the flow rule have been assumed. Equation (5.228), therefore can be highly non-linear in  $\mathbf{G}$ . Our problem is the determination of  $\{\mathbf{a}, \mathbf{G}, \zeta, U\}$  for a given thermodynamic state at the wave, a fixed normal  $\mathbf{N}$  and known values of the derivatives of the state variables ahead of the wave. These are fourteen unknowns, for which we will need equal number of equations. The relation (5.228) provides us with nine equations. To these we append three relations from (5.190), which is rewritten below

$$\mathbf{j}^{-1}\mathbb{A}\mathbf{G} + \mathbf{Q}\mathbf{a} = \rho_r \tilde{U}^2 \mathbf{a}, \quad (5.229)$$

where  $\mathbb{A}$  and  $\mathbf{Q}$  are as given in equations (5.191) and (5.192), respectively. An additional relation at the wave surface is provided from the yield condition. Recall the general form of yield criteria assumed in (3.146):

$$F(\mathbf{C}_H, \boldsymbol{\alpha}, \eta) = 0, \quad (5.230)$$

using which the following jump condition can be obtained

$$\llbracket F \rrbracket = 0. \quad (5.231)$$

Equations (5.228), (5.229), (5.231), and (5.177) are fourteen in number, which, at least in principle, can be solved for the fourteen unknowns mentioned above. Further

analytical study warrants specific constitutive assumptions. In the following we assume associative flow rules and consider two cases. In the first case we assume absence of hardening, and in the second case we consider hardening but only under an isothermal plastic flow. Moreover, we assume small elastic strains in both of these cases.

Case (i). We assume that the tensor functions  $\mathcal{P}$  and  $\mathbf{M}$  appearing in (5.221) and the scalar function  $F$  in (5.230) are all independent of  $\boldsymbol{\alpha}$  and  $\nabla\eta\mathbf{K}$ . As an immediate consequence, we note that the relation (5.231) is trivially satisfied.

For an associated plastic flow, the flow rule is of the form ( $\sigma \in \mathbb{R}$ )

$$\dot{\mathbf{K}}^{-1}\mathbf{K} = \sigma F_{\mathbf{C}_H}, \quad (5.232)$$

where the right hand side can be obtained from (4.30) and the chain rule. On the other hand, we have from (5.230)

$$F_{\mathbf{C}_H} \cdot \dot{\mathbf{C}}_H + F_\eta \dot{\eta} = 0. \quad (5.233)$$

Substitute  $\dot{\mathbf{C}}_H$  and  $\dot{\eta}$  from (5.222) and (5.171)<sub>1</sub>, respectively, into this equation to get

$$2F_{\mathbf{C}_H} \cdot (\mathbf{H}^T \dot{\mathbf{F}}\mathbf{K} - \mathbf{C}_H \dot{\mathbf{K}}^{-1}\mathbf{K}) - \frac{F_\eta}{\rho_r \theta} \mathbf{E}' \cdot \dot{\mathbf{K}}^{-1}\mathbf{K} = 0. \quad (5.234)$$

Assume that for small elastic strain,  $F_{\mathbf{C}_H} = O(|\boldsymbol{\epsilon}|)$ , where  $2\boldsymbol{\epsilon} = (\mathbf{C}_H - \mathbf{1})$  is such that  $|\boldsymbol{\epsilon}| \ll 1$ . Furthermore,  $\mathbf{H} = \mathbf{R} + O(|\boldsymbol{\epsilon}|)$  ( $\mathbf{R}$  is the rotation the polar decomposition of  $\mathbf{H}$ ),  $\mathbf{C}_H = \mathbf{1} + O(|\boldsymbol{\epsilon}|)$ , and  $\mathbf{E}' = \mathbf{S} + o(|\boldsymbol{\epsilon}|)$ . The last of these follow from (3.77) and (5.201)<sub>1</sub>.

Under the assumption of small elastic strain, equation (5.234) then reduces to

$$F_\boldsymbol{\epsilon} \cdot (\mathbf{R}^T \dot{\mathbf{F}}\mathbf{K} - \dot{\mathbf{K}}^{-1}\mathbf{K}) - \frac{F_\eta}{\rho_r \theta} \mathbf{S} \cdot \dot{\mathbf{K}}^{-1}\mathbf{K} \approx 0, \quad (5.235)$$

where we have used the chain rule to replace  $2F_{\mathbf{C}_H}$  by  $F_\boldsymbol{\epsilon}$ . Rearrange (5.235) to obtain

$$\left( F_\boldsymbol{\epsilon} + \frac{F_\eta}{\rho_r \theta} \mathbf{S} \right) \cdot \dot{\mathbf{K}}^{-1}\mathbf{K} \approx \mathbf{R} F_\boldsymbol{\epsilon} \mathbf{K}^T \cdot \dot{\mathbf{F}}. \quad (5.236)$$

Eliminating  $\mathbf{K}^{-1}\dot{\mathbf{K}}$  between (5.232) and (5.236) then yields

$$\sigma \approx \frac{2}{\left(F_{\boldsymbol{\epsilon}} + \frac{F_{\eta}}{\rho_r \theta} \mathbf{S}\right) \cdot F_{\boldsymbol{\epsilon}}} \mathbf{R}F_{\boldsymbol{\epsilon}}\mathbf{K}^T \cdot \dot{\mathbf{F}}, \quad (5.237)$$

where the denominator is assumed to be non zero. Substituting this expression for  $\sigma$  back into (5.232) we obtain

$$\mathbf{K}^{-1}\dot{\mathbf{K}} \approx \phi(F_{\boldsymbol{\epsilon}} \otimes \mathbf{R}F_{\boldsymbol{\epsilon}}\mathbf{K}^T)[\dot{\mathbf{F}}], \quad \text{where } \phi = \frac{1}{\left(F_{\boldsymbol{\epsilon}} + \frac{F_{\eta}}{\rho_r \theta} \mathbf{S}\right) \cdot F_{\boldsymbol{\epsilon}}}. \quad (5.238)$$

Note that the relation (5.238)<sub>1</sub> is a special case of (5.227)<sub>1</sub>, and the invertibility requirement for  $\mathcal{Q}$  in the general case reduces down to the assumption of a finite  $\phi$  in (5.238)<sub>2</sub> above. Comparing with (5.238)<sub>1</sub> with (5.227)<sub>1</sub>, we find that  $\mathcal{T} = \phi(F_{\boldsymbol{\epsilon}} \otimes \mathbf{R}F_{\boldsymbol{\epsilon}}\mathbf{K}^T)$  and as a consequence of our premise of no hardening,  $\llbracket \mathcal{T} \rrbracket = \mathbf{0}$ . The relation (5.228) thus becomes

$$\mathbf{G}\mathbf{K} \approx \phi(F_{\boldsymbol{\epsilon}} \otimes \mathbf{R}F_{\boldsymbol{\epsilon}}\mathbf{K}^T)[\mathbf{a} \otimes \mathbf{N}] \quad (5.239)$$

or with some rearrangement

$$\mathbf{G} \approx \phi(F_{\boldsymbol{\epsilon}}\mathbf{K}^{-1} \otimes \mathbf{R}F_{\boldsymbol{\epsilon}}\mathbf{K}^T)[\mathbf{a} \otimes \mathbf{N}] \quad (5.240)$$

which expresses a linear relation between  $\mathbf{G}$  and  $\mathbf{a}$  (Recall that,  $\mathbf{G}$  and  $\mathbf{a}$  denote the jump in rate of plastic distortion and the jump in the gradient of deformation gradient, respectively).

To obtain  $\mathbf{a}$ , we use (5.239) to substitute for  $\mathbf{G}$  in (5.190). The tensors  $\mathbb{A}$  and  $\mathbf{Q}$  appearing in (5.190) and defined in (5.191) and (5.192), reduce to the following form for small elastic strain: (use (5.201))

$$\mathbb{A}_{ijk} \approx -R_{il}\mathbb{C}_{lmqj}N_m^i K_{kq}, \quad \text{and} \quad (5.241)$$

$$Q_{ij} \approx R_{il}R_{jn}\mathbb{C}_{lkmn}N_k^i N_m^j, \quad (5.242)$$



where  $\mathbb{C}$  is the fourth order elasticity tensor defined in (5.199) and  $\mathbf{jN}^i = \mathbf{K}^T \mathbf{N}$  (cf. (5.186) and (5.187)). Also, rewrite  $\mathbf{G}$  from (5.240) in terms of indices as

$$G_{jk} \approx \mathbf{j}\phi \tilde{a}_r N_t^i (F\boldsymbol{\epsilon})_{rt} (F\boldsymbol{\epsilon})_{js} K_{sk}^{-1}, \quad \text{where } \tilde{\mathbf{a}} = \mathbf{R}^T \mathbf{a}. \quad (5.243)$$

Combining this with  $\mathbb{A}$  from (5.241) we get

$$\mathbb{A}_{ijk} G_{jk} \approx \mathbf{j}\phi R_{il} \mathbb{C}_{lmqj} N_t^i N_m^i (F\boldsymbol{\epsilon})_{rt} (F\boldsymbol{\epsilon})_{jq} \tilde{a}_r. \quad (5.244)$$

Substitute this in (5.190) and use (5.243)<sub>2</sub> to obtain

$$\phi \mathbb{C}_{lmqj} (F\boldsymbol{\epsilon})_{nk} (F\boldsymbol{\epsilon})_{jq} N_k^i N_m^i \tilde{a}_n + \mathbb{C}_{lkmn} N_k^i N_m^i \tilde{a}_n = \rho_r \tilde{U}^2 \tilde{a}_l. \quad (5.245)$$

This can be written as

$$Q_{ij}^p \tilde{a}_j = \rho_r \tilde{U}^2 \tilde{a}_i, \quad (5.246)$$

where

$$Q_{ln}^p = \phi \mathbb{C}_{lmqj} (F\boldsymbol{\epsilon})_{nk} (F\boldsymbol{\epsilon})_{jq} N_k^i N_m^i + \mathbb{C}_{lkmn} N_k^i N_m^i \quad (5.247)$$

is the plastic acoustic tensor. The positive (and real) eigen values of  $\mathbf{Q}^p$  correspond to real speeds of the plastic acceleration wave. Unlike the elastic acoustic tensor, the plastic acoustic tensor might be non-symmetric. Specific forms of the yield criteria are now required for any further analysis of the wave speeds and amplitude. Once wave speeds and amplitudes are obtained, the corresponding values of  $\mathbf{G}$  and  $\zeta$  can be calculated using (5.240) and (5.177), respectively. Finally, note that even though we have assumed hardening to be absent, a jump in the total dislocation density persists and can be obtained from the compatibility condition (5.167).

Case (ii). We would now like to consider the presence of hardening (through dislocation density) in an associated (isothermal) flow rule and an isothermal yield criteria. The flow rule is assumed as (cf. (4.30))

$$\dot{\mathbf{K}}^{-1}\mathbf{K} = \sigma F_{\mathbf{C}_H}, \quad (5.248)$$

where  $\sigma \in \mathbb{R}$  is a scalar valued function of  $\{\dot{\mathbf{C}}_H, \mathbf{C}_H, \boldsymbol{\alpha}\}$  and (cf. (5.230))

$$F(\mathbf{C}_H, \boldsymbol{\alpha}) = 0, \quad (5.249)$$

defines the yield criterion. Moreover, comparing (5.248) with (5.221), we note that there exists a tensor  $\mathbf{J}$  such that  $\sigma = \mathbf{J} \cdot \dot{\mathbf{C}}_H$ , with  $\mathbf{J} = \mathbf{J}(\mathbf{C}_H, \boldsymbol{\alpha})$  (cf. (4.56), where an expression for  $\mathbf{J}$  has also been derived), thus reducing (5.248) to

$$\dot{\mathbf{K}}^{-1}\mathbf{K} = (F_{\mathbf{C}_H} \otimes \mathbf{J})[\dot{\mathbf{C}}_H]. \quad (5.250)$$

Therefore, the tensor  $\mathcal{P}$  in (5.221) is now given by  $(F_{\mathbf{C}_H} \otimes \mathbf{J})$ . As a result, the tensor  $\mathcal{Q}$  in (5.225) reduces to

$$\mathcal{Q} = \mathbb{I} + F_{\boldsymbol{\epsilon}} \otimes \mathbf{C}_H \mathbf{J}, \quad (5.251)$$

where we have also used elastic strain  $\boldsymbol{\epsilon}$  and chain rule to replace  $F_{\mathbf{C}_H}$  by  $F_{\boldsymbol{\epsilon}}$  ( $F$  is now understood to be a function of  $\boldsymbol{\epsilon}$  (and  $\boldsymbol{\alpha}$ ) rather than  $\mathbf{C}_H$ ). Assuming  $F_{\boldsymbol{\epsilon}} = O(|\boldsymbol{\epsilon}|)$ ,  $\mathbf{J} = O(1)$ , and noting that  $\mathbf{C}_H = \mathbf{1} + O(|\boldsymbol{\epsilon}|)$ , equation (5.251) for small elastic strains yields

$$\mathcal{Q} \approx \mathbb{I} + F_{\boldsymbol{\epsilon}} \otimes \mathbf{J}. \quad (5.252)$$

Moreover, the tensor  $\mathcal{R}$  in (5.226) now takes the form

$$\mathcal{R} \approx F_{\boldsymbol{\epsilon}} \otimes \mathbf{R} \mathbf{J} \mathbf{K}. \quad (5.253)$$

Next, to write (5.250) in the form (5.227)<sub>1</sub>, we need to evaluate the inverse of  $\mathcal{Q}$ . We obtain<sup>9</sup>

$$\mathcal{Q}^{-1} \approx \mathbb{I} - \frac{F_{\boldsymbol{\epsilon}} \otimes \mathbf{J}}{1 + F_{\boldsymbol{\epsilon}} \cdot \mathbf{J}}, \quad (5.254)$$

assuming that  $(1 + F_{\boldsymbol{\epsilon}} \cdot \mathbf{J}) \neq 0$ . The tensor  $\mathcal{T}$  in (5.227)<sub>2</sub> can then be evaluated as

$$\mathcal{T} = \mathcal{Q}^{-1} \mathcal{R} \approx \left( \mathbb{I} - \frac{F_{\boldsymbol{\epsilon}} \otimes \mathbf{J}}{1 + F_{\boldsymbol{\epsilon}} \cdot \mathbf{J}} \right) (F_{\boldsymbol{\epsilon}} \otimes \mathbf{RJK}) \quad (5.255)$$

$$= \frac{F_{\boldsymbol{\epsilon}} \otimes \mathbf{RJK}}{1 + F_{\boldsymbol{\epsilon}} \cdot \mathbf{J}}. \quad (5.256)$$

it should be noted that  $\mathcal{T}$  will be discontinuous across the wave. This is because the tensors  $F_{\boldsymbol{\epsilon}}$  and  $\mathbf{J}$  depend on  $\boldsymbol{\alpha}$ , which is discontinuous across the wave surface. Substitute  $\mathcal{T}$  into (5.228) yields an equation, which combined with (5.229) and (5.231), give us a complete set of governing equations, sufficient to obtain our unknowns.

*Remark 5.3.1.* (Unloading plastic wave) For an unloading plastic acceleration wave, plasticity evolves only in its front (which is the direction into which wave propagates), i.e.  $\dot{\mathbf{K}}^+ \neq \mathbf{0}$  but  $\dot{\mathbf{K}}^- = \mathbf{0}$ . Since  $\dot{\mathbf{K}}^+$  is assumed to be known,  $\mathbf{G}$  follows directly from (5.164)<sub>2</sub> as

$$\mathbf{G} = -\frac{1}{U} (\mathbf{K}^{\dot{-}1})^+. \quad (5.257)$$

This can then be substituted into (5.189) to get

$$-\frac{1}{j^2 \tilde{U}} \mathbb{A}[(\mathbf{K}^{\dot{-}1})^+] + \mathbf{Qa} = \rho_r \tilde{U}^2 \mathbf{a}. \quad (5.258)$$

---

<sup>9</sup>For a fourth order tensor of the form

$$\mathcal{A}_{rmpq} = \mathbb{I}_{rmpq} + M_{rm} N_{pq},$$

we have

$$\mathcal{A}_{rmpq}^{-1} = \mathbb{I}_{rmpq} - \frac{M_{rm} N_{pq}}{1 + M_{ij} N_{ij}},$$

where the second order tensors  $\mathbf{M}$  and  $\mathbf{N}$  are arbitrary but satisfy the condition  $(1 + \mathbf{M} \cdot \mathbf{N}) \neq 0$ . The result can be verified by a direct substitution.

Note that if the tensor  $(\mathbf{Q} - \rho_r \tilde{U}^2 \mathbf{1})$  is not invertible, then  $\det(\mathbf{Q} - \rho_r \tilde{U}^2 \mathbf{1}) = 0$  and the problem is reduced to elastic acceleration waves. To obtain a solution for plastic waves, however, we assume that  $(\mathbf{Q} - \rho_r \tilde{U}^2 \mathbf{1})$  is invertible. It then follows from (5.258) that

$$\mathbf{a} = \frac{1}{j^2 \tilde{U}} (\mathbf{Q} - \rho_r \tilde{U}^2 \mathbf{1})^{-1} \mathbb{A}[(\mathbf{K}^{-1})^+]. \quad (5.259)$$

In (5.259) everything on the right hand side is known, except for the wave speed. To obtain the wave speed, recall the yield criteria, which holds immediately ahead of the wave: (cf. (5.230))

$$F^+ = 0. \quad (5.260)$$

This equality can also be viewed as the equation for surface  $S_t$ , i.e. as  $S_t = \{\mathbf{X} \in \kappa_r : F^+(\mathbf{X}, t) = 0\}$ . The wave speed can then be computed via the relation (cf. (2.49))

$$U = -\frac{(F^+)_t}{|\nabla F^+|}. \quad (5.261)$$

This can then be substituted back into (5.259) to solve for  $\mathbf{a}$  (Also use  $\tilde{U} = j^{-1}U$ , with  $j$  from (5.187)<sub>2</sub>). The evaluation of  $U$  using this method was first considered by Green [63].

*Remark 5.3.2.* (Rate dependent plastic flow) For a special class of rate dependent flow rules, we find that the governing equations decouple themselves. Consider the flow rules of the type (cf. (5.193))

$$\dot{\mathbf{K}}^{-1} \mathbf{K} = \mathbf{D}(\mathbf{C}_H, \boldsymbol{\alpha}, \eta, \nabla \eta \mathbf{K}), \quad (5.262)$$

which then implies

$$-U \mathbf{G} \mathbf{K} = \llbracket \mathbf{D} \rrbracket. \quad (5.263)$$

Equation (5.263) is a special case of (5.194), differing in the fact that  $\llbracket \mathbf{D} \rrbracket$ , unlike the general case, has no dependence on  $\mathbf{a}$ . Contrasting this to the analogous relation for the

rate independent case, i.e. (5.227), we note that in the considered class of rate dependent flow rules, we have decoupled equations for  $\mathbf{G}$  and  $\mathbf{a}$ . Although complicated, (5.263) should be seen as the set of equations which determine  $\mathbf{G}$ . Once  $\mathbf{G}$  is obtained, it can be substituted in (5.190) to solve for  $\mathbf{a}$  and  $\zeta$ .

## Chapter 6

# Interfacial Plastic Flow

In this last chapter we are concerned with the plastic flow at the interface, which is endowed with an independent (from the bulk) constitutive structure. The motivation is derived from the problems where plasticity evolves not only in the three dimensional bulk, but also along the two dimensional interface. The resulting coupling of these two mechanisms drives the interface as well as the dislocation content in the bulk. Historically, the impetus for studying interfaces, particularly in metals, came from the seminal work by Smith [159], who presented many experimental observations as well as simple mathematical models. Immediately much research work followed, exposing many interesting problems in the area of interface mechanics in solids [17, 58, 150]. A more detailed review can be accessed from the books by Howe [77], Gottstein & Shvindlerman [59], and Sutton & Balluffi [161].

In Section 6.1 we obtain the restrictions on constitutive functions, defined on the interface, on using their invariance under compatible changes in the reference configuration. A corresponding representation theorem for the material points in the bulk was obtained in

Section 3.3. In the context of singular surfaces, the concept of a compatible change in the reference configuration was introduced in our discussion on an invariant measure of surface dislocation density in Subsection 5.1.2. Such an invariance is to be naturally expected of the constitutive functions, which should not depend on our choice of a reference configuration. We show that constitutive functions can depend on plastic distortion only through the true surface dislocation density. A dependence on plastic distortion is also possible as suitable coefficients to the rate terms: plastic distortion rate and the interface velocity.

In Section 6.2, we start by recalling the consequences of the dissipation inequality as discussed earlier in Chapters 2 and 3. We go on to extend the discussion of dissipation inequality and its consequences by adding interface stress and interface energy into the formulation. Added mechanisms of dissipation now appear, which couple with each other in the evolution of the dynamics of the concerned problem. The resulting theory provides, for example, the basic framework for studying the problem of accompanying plastic deformation during grain/phase boundary migration. Most of the previous work in the subject has been restricted to coherent interfaces in an elastically deforming solid, see for example the reviews by Fried & Gurtin [55] and Fischer et al. [51] (and the references therein). With regard to incoherent interfaces, the work has been restricted to interfaces bounded by bulk with no dislocation content [98, 105, 29]. In these earlier frameworks, it is not possible to model the coupling of plastic flow in the bulk and the interface. Our formulation however, extends their treatment to incoherent interfaces which are bounded by dislocated bulk.

We end the chapter with a long remark on the interface energy. We use the basic invariant properties to deduce restrictions on its form. The aim of this remark is to clearly

present the concept of strain energy, which otherwise remains shrouded with mystery in most of the scientific literature.

## 6.1 Invariance under compatible changes in the reference configuration

As motivated in Section 3.3, our constitutive functions should be such that they are invariant with respect to any compatible change in the reference configuration. This argument is based on the fact that the material response should be independent of any choice of the reference configuration. A compatible change in the configuration ensures that the topological structure of the reference configuration remains unaltered. Consider two reference configurations,  $\kappa_{r_1}$  and  $\kappa_{r_2}$  with a map  $\boldsymbol{\lambda}$  such that  $\mathbf{X}_2 = \boldsymbol{\lambda}(\mathbf{X}_1)$ , where  $\mathbf{X}_1 \in \kappa_{r_1}$  and  $\mathbf{X}_2 \in \kappa_{r_2}$ , with invertible gradient  $\mathbf{A} = \nabla_1 \boldsymbol{\lambda}$  (such that  $\mathbf{K}_2 = \mathbf{A}\mathbf{K}_1$ ). For  $\mathbf{A}$  to be a compatible deformation from  $\kappa_{r_1}$  and  $\kappa_{r_2}$ , the Hadamard's rank one compatibility  $[[\mathbf{A}]] = \mathbf{d} \otimes \mathbf{N}$ , where  $\mathbf{d} \in \mathcal{V}$  is arbitrary, holds at the singular interface. Such a compatible transformation leaves the Burgers vector invariant for any closed curve cutting across the singular surface. This was proved earlier in Subsection 5.1.2. The following transformation rules can then be inferred for elastic and plastic distortions (and their rates):

$$\mathbf{K}_2^\pm = \mathbf{A}^\pm \mathbf{K}_1^\pm, \quad \mathbf{H}_2^\pm = \mathbf{H}_1^\pm, \quad \text{and} \quad (6.1)$$

$$\dot{\mathbf{K}}_2^\pm = \mathbf{A}^\pm \dot{\mathbf{K}}_1^\pm, \quad \dot{\mathbf{H}}_2^\pm = \dot{\mathbf{H}}_1^\pm. \quad (6.2)$$

We would also require the transformation rules for surface permutation tensor  $\boldsymbol{\varepsilon}_{(\mathbf{N})}$ , surface dislocation density  $\boldsymbol{\beta}_{r_2}$ , and referential surface speed  $U$ . Two of these transformation rules



were obtained earlier in Subsection 5.1.2 (cf. (5.38) and (5.40)). We restate them below:

$$\boldsymbol{\varepsilon}_{(\mathbf{N}_2)} = (j_A)^{-1} \mathbf{A}^\pm \boldsymbol{\varepsilon}_{(\mathbf{N}_1)} (\mathbf{A}^\pm)^T, \quad (6.3)$$

$$\boldsymbol{\beta}_{r_2}^T \mathbb{P}_2 = (j_A)^{-1} \boldsymbol{\beta}_{r_1}^T \mathbb{P}_1 (\mathbf{A}^\pm)^T, \quad (6.4)$$

where  $j_A = \frac{dA_2}{dA_1}$  is the ratio of infinitesimal areas corresponding to  $S_{t_2}$  and  $S_{t_1}$ . These relation can be used to obtain an invariant form of surface permutation tensor and surface dislocation density. Such invariant forms is independent of any compatible changes in the reference configuration. They follow from equations (6.3) and (6.4) on noting that

$$\mathbf{A}^\pm = \mathbf{K}_2^\pm (\mathbf{K}_1^\pm)^{-1}, \quad \text{and } j_A = \frac{j_2^\pm}{j_1^\pm}, \quad (6.5)$$

where  $j_a^\pm$  ( $a = 1, 2$ ) represents the ratio of infinitesimal area elements (of the singular surface) in the reference and the intermediate configuration. At this point, it would be helpful to recall that the tangent plane at the singular surface, in the reference and the current configuration, is mapped locally into two tangential planes in the intermediate configuration. It is for this reason that we have two measures of the ratio of infinitesimal areas in the reference and intermediate configuration, for e.g.  $j_1^\pm$ . Substituting (6.5) into (6.3) and (6.4), we obtain

$$j_2^\pm (\mathbf{K}_2^\pm)^{-1} \boldsymbol{\varepsilon}_{(\mathbf{N}_2)} (\mathbf{K}_2^\pm)^{-1} = j_1^\pm (\mathbf{K}_1^\pm)^{-1} \boldsymbol{\varepsilon}_{(\mathbf{N}_1)} (\mathbf{K}_1^\pm)^{-T}, \quad \text{and} \quad (6.6)$$

$$j_2^\pm \boldsymbol{\beta}_{r_2}^T \mathbb{P}_2 (\mathbf{K}_2^\pm)^{-1} = j_1^\pm \boldsymbol{\beta}_{r_1}^T \mathbb{P}_1 (\mathbf{K}_1^\pm)^{-T}, \quad (6.7)$$

respectively. Define

$$\boldsymbol{\varepsilon}^\pm = j^\pm (\mathbf{K}^\pm)^{-1} \boldsymbol{\varepsilon}_{(\mathbf{N})} (\mathbf{K}^\pm)^{-1}, \quad \text{and} \quad (6.8)$$

$$(\boldsymbol{\beta}^\pm)^T = j^\pm \boldsymbol{\beta}_r^T \mathbb{P} (\mathbf{K}^\pm)^{-T}, \quad (6.9)$$

where  $j^\pm$  represents the ratio of infinitesimal area elements (of the singular surface) in any reference and intermediate configuration. We call the quantities  $\boldsymbol{\varepsilon}^\pm$  and  $\boldsymbol{\beta}^\pm$ , the true surface permutation tensor and true surface dislocation density (cf. 5.43), respectively. Both of these are invariant with respect to any compatible change in the reference configuration.

Next, we would like to obtain the transformation for  $U$ . Start by recalling its definition from (2.49), i.e.

$$U_1 = -\frac{\dot{\phi}}{|\nabla_1 \phi|}, \quad \text{where } \phi(\mathbf{X}_1, t) = 0 \quad (6.10)$$

determines the singular surface  $S_{t1}$  in the reference configuration  $\kappa_{r1}$ . The singular surface in the reference configuration  $\kappa_{r2}$  is then given by

$$\hat{\phi}(\mathbf{X}_2, t) = \phi(\boldsymbol{\lambda}^{-1}(\mathbf{X}_2), t) = 0. \quad (6.11)$$

The normal speed in the reference configuration  $\kappa_{r2}$  is then given by

$$U_2 = -\frac{\dot{\hat{\phi}}}{|\nabla_2 \hat{\phi}|}. \quad (6.12)$$

To relate  $U_1$  and  $U_2$ , we start by noting the following identities:

$$\dot{\hat{\phi}} = \dot{\phi}, \quad \text{and } \nabla_2 \hat{\phi} = (\mathbf{A}^\pm)^{-T} \nabla_1 \phi, \quad (6.13)$$

where (6.13)<sub>2</sub> follows from (6.11)<sub>1</sub> on using the chain rule of differentiation. Further, use the definition of the normal (cf. (2.49)) and Nanson's formula, given by

$$\mathbf{N}_1 = \frac{\nabla_1 \phi}{|\nabla_1 \phi|}, \quad \mathbf{N}_2 = \frac{\nabla_2 \hat{\phi}}{|\nabla_2 \hat{\phi}|}, \quad \text{and } \mathbf{N}_2 = j_A^{-1}(\mathbf{A}^\pm)^* \mathbf{N}_1, \quad (6.14)$$

to obtain

$$\frac{|\nabla_2 \phi|}{|\nabla_1 \hat{\phi}|} = j_A J_{A^\pm}^{-1}. \quad (6.15)$$

Combining relations (6.15), (6.13)<sub>1</sub>, (6.10)<sub>1</sub>, and (6.12), we get

$$U_2 = U_1 j_A^{-1} J_{A^\pm}. \quad (6.16)$$

Moreover, use (6.5) to get

$$j_2^\pm J_{K_2^\pm}^{-1} U_2 = j_1^\pm J_{K_1^\pm}^{-1} U_1, \quad (6.17)$$

thus defining

$$\hat{U}^\pm = j^\pm J_{K^\pm}^{-1} U \quad (6.18)$$

as the true normal speeds associated with the singular interface.

We now use these transformation rules to obtain the representation for functions to be invariant under compatible changes in the reference configuration. A scalar function  $f = \hat{f}(\mathbf{H}_1^\pm, \mathbf{K}_1^\pm, \dot{\mathbf{H}}_1^\pm, \dot{\mathbf{K}}_1^\pm, U)$  is invariant under the change in reference configuration from  $\kappa_{r_1}$  to  $\kappa_{r_2}$  if

$$\hat{f}(\mathbf{H}_1^\pm, \mathbf{K}_1^\pm, \dot{\mathbf{H}}_1^\pm, \dot{\mathbf{K}}_1^\pm, U_1) = \hat{f}(\mathbf{H}_2^\pm, \mathbf{K}_2^\pm, \dot{\mathbf{H}}_2^\pm, \dot{\mathbf{K}}_2^\pm, U_2), \quad (6.19)$$

where the variables are related to each other as in (6.1), (6.2), and (6.16). The choice of arguments for the function  $f$  is motivated from the variables appearing in the dissipation inequality in the next section. To obtain a necessary condition for (6.19) to hold true, let  $\mathbf{A}^+ = (\mathbf{K}_1^+)^{-1}$  and  $\mathbf{A}^- = (\mathbf{K}_1^-)^{-1} - \boldsymbol{\beta}_{r_1}^T \boldsymbol{\varepsilon}_{(\mathbf{N}_1)}$  locally at the point at which (6.19) is evaluated. This choice indeed satisfies the rank one jump restriction for  $\mathbf{A}$ , as can be verified from the jump condition (5.6) for  $\mathbf{K}^{-1}$ . With this choice for  $\mathbf{A}^\pm$  we can use (6.1), (6.2), and (6.16)

to obtain the following:

$$\mathbf{K}_2^+ = \mathbf{1}, \quad \mathbf{K}_2^- = \mathbf{1} - \beta_{r_1}^T \boldsymbol{\varepsilon}_{(\mathbf{N}_1)} \mathbf{K}_1^-, \quad (6.20)$$

$$\dot{\mathbf{K}}_2^+ = (\mathbf{K}_1^+)^{-1} \dot{\mathbf{K}}_1^+, \quad \dot{\mathbf{K}}_2^- = (\mathbf{K}_1^-)^{-1} \dot{\mathbf{K}}_1^- - \beta_{r_1}^T \boldsymbol{\varepsilon}_{(\mathbf{N}_1)} \dot{\mathbf{K}}_1^-, \quad \text{and} \quad (6.21)$$

$$U_2 = U_1 j_1^+ J_{\mathbf{K}_1^+}^{-1}. \quad (6.22)$$

Therefore, a necessary condition for  $f$  to be invariant is to have the representation

$$f = \tilde{f}(\mathbf{H}^\pm, \beta_r^T \boldsymbol{\varepsilon}_{(\mathbf{N})} \mathbf{K}^-, \dot{\mathbf{H}}^\pm, (\mathbf{K}^\pm)^{-1} \dot{\mathbf{K}}^\pm, \hat{U}^+), \quad (6.23)$$

where  $\hat{U}^+$  is given in (6.18). For  $f$  to be invariant under arbitrary transformations, it has to satisfy

$$\tilde{f}(\mathbf{H}_1^\pm, \beta_{r_1}^T \boldsymbol{\varepsilon}_{(\mathbf{N}_1)} \mathbf{K}_1^\pm, \dot{\mathbf{H}}_1^\pm, (\mathbf{K}_1^\pm)^{-1} \dot{\mathbf{K}}_1^\pm, \hat{U}^+) = \tilde{f}(\mathbf{H}_2^\pm, \beta_{r_2}^T \boldsymbol{\varepsilon}_{(\mathbf{N}_2)} \mathbf{K}_2^\pm, \dot{\mathbf{H}}_2^\pm, (\mathbf{K}_2^\pm)^{-1} \dot{\mathbf{K}}_2^\pm, \hat{U}^+). \quad (6.24)$$

It is easy to see that all the arguments of  $\tilde{f}$  are invariant under arbitrary  $\mathbf{A}$ , except for  $\beta_{r_2}^T \boldsymbol{\varepsilon}_{(\mathbf{N}_2)} \mathbf{K}_2^-$ , which can be expanded using (6.1)<sub>1</sub>, (6.3), and (6.4) to get

$$\begin{aligned} \beta_{r_2}^T \boldsymbol{\varepsilon}_{(\mathbf{N}_2)} \mathbf{K}_2^- &= \beta_{r_2}^T \mathbb{P}_2 \boldsymbol{\varepsilon}_{(\mathbf{N}_2)} \mathbf{K}_2^- \\ &= (j_A)^{-2} \beta_{r_1}^T \mathbb{P}_1 (\mathbf{A}^-)^T \mathbf{A}^- \boldsymbol{\varepsilon}_{(\mathbf{N}_1)} (\mathbf{A}^-)^T \mathbf{A}^- \mathbf{K}_1^-. \end{aligned} \quad (6.25)$$

Choose  $\mathbf{A}^- = (\mathbf{K}_1^-)^{-1}$  (any value can be taken for  $\mathbf{A}^+$  as long as  $\llbracket \mathbf{A} \rrbracket$  is rank one). Obtain

$$\beta_{r_2}^T \boldsymbol{\varepsilon}_{(\mathbf{N}_2)} \mathbf{K}_2^- = (\beta^-)^T \boldsymbol{\varepsilon}_{(\mathbf{N})}^-, \quad (6.26)$$

where the terms on right hand side are defined in equations (6.8) and (6.9).

The choice of a particular sign in the above discussion is arbitrary. Consequently, we obtain the necessary and sufficient form of the representation for  $f$  to be invariant under

compatible changes in the reference configuration as

$$f = \check{f}(\mathbf{H}^\pm, (\boldsymbol{\beta}^\pm)^T \boldsymbol{\varepsilon}_{(\mathbf{N})}^\pm, \dot{\mathbf{H}}^\pm, (\mathbf{K}^\pm)^{-1} \dot{\mathbf{K}}^\pm, \hat{U}^\pm). \quad (6.27)$$

## 6.2 Thermodynamics: dissipation inequality

The mechanical version of second law of thermodynamics (under isothermal temperature field) can be stated as (with zero body force):

$$\text{Dissipation } D \doteq \int_{\partial\Omega} \mathbf{P}\mathbf{N} \cdot \mathbf{v} dA - \frac{d}{dt} \int_{\Omega} \Psi dV \geq 0, \quad (6.28)$$

where  $D$  is the dissipation associated with  $\Omega \subset \kappa_i$ . Before discussing the case with interface energy, we recall our discussion from Chapter 3 and also discuss a case with diffusion.

**Case 1** We assume all fields to be sufficiently smooth on  $\Omega$ . We allow body to deform elastic-plastically in the bulk. We can write the free energy density (including kinetic energy) per unit volume of the reference configuration as

$$\Psi = J_K^{-1} W(\mathbf{H}) + \frac{1}{2} \rho_\kappa \mathbf{v} \cdot \mathbf{v}, \quad (6.29)$$

where  $\rho_\kappa$  is the density in reference configuration. Substituting (6.29) in (6.28) for a smooth and fixed  $\Omega$  we obtain

$$(J_K^{-1} W(\mathbf{H}) \mathbf{1} - \mathbf{F}^T \mathbf{P}) \cdot \dot{\mathbf{K}} \mathbf{K}^{-1} \geq 0 \quad \text{in } \Omega, \quad (6.30)$$

where we have used the equilibrium relation ( $\text{Div } \mathbf{P} = \rho_\kappa \dot{\mathbf{v}}$ ) and the arbitrariness of  $\Omega$ .

**Case 2** There exists a surface  $S = S_t \cap \Omega \neq \emptyset$  inside  $\Omega$ , across which various fields suffer jump discontinuities. The surface is assumed to be moving with an velocity  $U \mathbf{N}_s$ , where

$\mathbf{N}_s$  denotes the normal to the surface  $S$ . In such a case

$$\int_{\partial\Omega} \mathbf{P}\mathbf{N} \cdot \mathbf{v}dA = \int_{\Omega} \text{Div}(\mathbf{P}^T \mathbf{v})dV + \int_S \llbracket \mathbf{P}^T \mathbf{v} \rrbracket \cdot \mathbf{N}_s dA \quad (6.31)$$

and

$$\frac{d}{dt} \int_{\Omega} \Psi dV = \int_{\Omega} \dot{\Psi} dV - \int_S \llbracket \Psi \rrbracket U dA. \quad (6.32)$$

We first evaluate,

$$\begin{aligned} \llbracket \mathbf{P}^T \mathbf{v} \rrbracket \cdot \mathbf{N}_s &= \llbracket \mathbf{P}^T \rrbracket \langle \mathbf{v} \rangle \cdot \mathbf{N}_s + \langle \mathbf{P}^T \rangle \llbracket \mathbf{v} \rrbracket \cdot \mathbf{N}_s \\ &= \llbracket \mathbf{P} \mathbf{N}_s \rrbracket \cdot \langle \mathbf{v} \rangle + \langle \mathbf{P} \rangle \cdot \llbracket \mathbf{v} \rrbracket \otimes \mathbf{N}_s \\ &= -\rho_{\kappa} U \llbracket \mathbf{v} \rrbracket \cdot \langle \mathbf{v} \rangle - U \langle \mathbf{P} \rangle \cdot \llbracket \mathbf{F} \rrbracket \\ &= -\frac{1}{2} \rho_{\kappa} U \llbracket \mathbf{v} \cdot \mathbf{v} \rrbracket - U \langle \mathbf{P} \rangle \cdot \llbracket \mathbf{F} \rrbracket, \end{aligned} \quad (6.33)$$

where in the third equality we have used  $\llbracket \mathbf{P} \rrbracket \mathbf{N}_s = -\rho_{\kappa} U \llbracket \mathbf{v} \rrbracket$  and  $-U \llbracket \mathbf{F} \rrbracket = \llbracket \mathbf{v} \rrbracket \otimes \mathbf{N}_s$ , which follow from the linear momentum balance and Hadamard's lemma, respectively (cf.

Chapter 2). Moreover, we can write

$$\mathbf{N}_s \cdot \llbracket \mathbf{F}^T \mathbf{P} \rrbracket \mathbf{N}_s = \langle \mathbf{P} \rangle \cdot \llbracket \mathbf{F} \rrbracket + \frac{1}{2} \rho_{\kappa} U^2 \mathbf{N}_s \cdot \llbracket \mathbf{F}^T \mathbf{F} \rrbracket \mathbf{N}_s, \quad (6.34)$$

where the last term is obtained using  $\llbracket \mathbf{P} \rrbracket \mathbf{N}_s = \rho_{\kappa} U^2 \llbracket \mathbf{F} \rrbracket \mathbf{N}_s$ . The second term follows from

the following:  $\mathbf{N}_s \cdot \llbracket \mathbf{F}^T \rrbracket \langle \mathbf{P} \rangle \mathbf{N}_s = \langle \mathbf{P} \rangle \cdot \llbracket \mathbf{F} \rrbracket (\mathbf{N}_s \otimes \mathbf{N}_s) = \langle \mathbf{P} \rangle \cdot \llbracket \mathbf{F} \rrbracket$ , where the last equality

is a consequence of Hadamard's lemma. Finally, substituting equations (6.31)-(6.34) into

(6.28) we obtain

$$\begin{aligned} & \int_{\Omega} (J_K^{-1} W(\mathbf{H}) \mathbf{1} - \mathbf{F}^T \mathbf{P}) \cdot \dot{\mathbf{K}} \mathbf{K}^{-1} dV \\ & + \int_S U \mathbf{N}_s \cdot (\llbracket J_K^{-1} W(\mathbf{H}) \mathbf{1} - \mathbf{F}^T \mathbf{P} \rrbracket + \frac{1}{2} \rho_{\kappa} U^2 \llbracket \mathbf{F}^T \mathbf{F} \rrbracket) \cdot \mathbf{N}_s dA \geq 0. \end{aligned} \quad (6.35)$$

Arbitrariness of  $\Omega$  and  $S$  then results into the following local relations:

$$(J_K^{-1}W(\mathbf{H})\mathbf{1} - \mathbf{F}^T\mathbf{P}) \cdot \dot{\mathbf{K}}\mathbf{K}^{-1} \geq 0 \quad \text{in } \Omega/S \quad (6.36)$$

and

$$U\mathbf{N}_s \cdot (\llbracket J_K^{-1}W(\mathbf{H})\mathbf{1} - \mathbf{F}^T\mathbf{P} \rrbracket + \frac{1}{2}\rho_\kappa U^2 \llbracket \mathbf{F}^T\mathbf{F} \rrbracket)\mathbf{N}_s \geq 0 \quad \text{on } S. \quad (6.37)$$

Note that unlike the case of elastically deforming bulk, here the flow in bulk is coupled to the flow at the surface of discontinuity.

**Case 3** We now consider the case allowing for mass transfer across the interface. The bulk on one side of the interface grows at the expense of the bulk on the other side of the interface. It can be deduced from the equation for balance of mass that the mass flux across unit area of the reference configuration is given by  $\rho_\kappa U$ . We assume that diffusion takes place only on the interface. We can then modify equation (6.28) to include working by the chemical potential  $\mu$  as

$$\text{Dissipation } D \doteq \int_{\partial\Omega} \mathbf{P}\mathbf{N} \cdot \mathbf{v}dA + \int_S \llbracket \mu \rrbracket \rho_\kappa U dA - \frac{d}{dt} \int_\Omega \Psi dV \geq 0. \quad (6.38)$$

If we further assume that the growth process is purely dissipative (provides no energy change), then the dissipation relation at the interface follows from equation (6.37) after a slight modification:

$$U\mathbf{N}_s \cdot (\llbracket J_K^{-1}W(\mathbf{H})\mathbf{1} + \rho\mu\mathbf{1} - \mathbf{F}^T\mathbf{P} \rrbracket + \frac{1}{2}\rho_\kappa U^2 \llbracket \mathbf{F}^T\mathbf{F} \rrbracket)\mathbf{N}_s \geq 0 \quad \text{on } S. \quad (6.39)$$

The inequality (6.36) in the bulk remains unchanged.

**Case 4** Consider now the case when the interface itself contributes energetically and is therefore endowed with an energy density (per unit area of the reference configuration),

say  $\phi$ . We would also need to include working due to interfacial stresses in the dissipation inequality. Before writing the the dissipation inequality, we deduce the interfacial Piola stress tensor.

The boundary of the interface  $S \in \Omega$  is denoted by  $\partial S$ . Let the unit normal to  $S$  be given by  $\mathbf{N}_s$ . Let the outward unit normal to  $\partial S$  (such that it is normal to  $\mathbf{N}_s$ ) be  $\hat{\nu}$  and the unit vector lying in the tangential space of  $\partial S$  be  $\hat{\mathbf{t}}$ . The triad of unit vectors  $\{\hat{\mathbf{t}}, \mathbf{N}_s, \hat{\nu}\}$  form an orthogonal system of vectors in the vector space of the reference configuration. A similar triad of unit vectors can be defined in the current configuration  $\omega$ , where the interface is denoted by  $s$  and its boundary by  $\partial s$ , with the outward unit normal given by  $\nu$  and a tangential vector  $\mathbf{t}$ . The orthogonal triad of unit vectors in the current configuration is then given by  $\{\mathbf{t}, \mathbf{n}_s, \nu\}$ .

If  $\mathbf{T}$  is the Cauchy stress tensor, acting on the interface  $s$ , then the net force

$$\int_{\partial s} \mathbf{T} \nu dl \quad (6.40)$$

acts on the boundary of the interface. By Nanson's formula we have,  $\mathbf{n}_s da = (\mathbf{F}^\pm)^* \mathbf{N}_s dA$ . Moreover,  $\mathbf{t} dl = \mathbf{F}^\pm \hat{\mathbf{t}} dL$ . It is easy to verify that  $\mathbf{t} \cdot \mathbf{n}_s = 0$  implies  $\hat{\mathbf{t}} \cdot \mathbf{N}_s = 0$ . Therefore, on using  $\nu = \mathbf{t} \times \mathbf{n}_s$  we can obtain

$$\nu dl = j_A^{-1} (\mathbf{F}^\pm \hat{\mathbf{t}} \times (\mathbf{F}^\pm)^* \mathbf{N}_s) dL, \quad (6.41)$$



where  $j_A = \frac{da}{dA}$ . Substituting  $\hat{\mathbf{t}} = \mathbf{N}_s \times \hat{\boldsymbol{\nu}}$  we get

$$\begin{aligned}
\nu dl &= j_A^{-1} (\mathbf{F}^\pm (\mathbf{N}_s \times \hat{\boldsymbol{\nu}}) \times (\mathbf{F}^\pm)^* \mathbf{N}_s) dL \\
&= j_A^{-1} J_F^{-1} (((\mathbf{F}^\pm)^* \mathbf{N}_s \times (\mathbf{F}^\pm)^* \hat{\boldsymbol{\nu}}) \times (\mathbf{F}^\pm)^* \mathbf{N}_s) dL \\
&= j_A^{-1} J_F^{-1} (((\mathbf{F}^\pm)^* \mathbf{N}_s \cdot (\mathbf{F}^\pm)^* \mathbf{N}_s) (\mathbf{F}^\pm)^* \hat{\boldsymbol{\nu}} - ((\mathbf{F}^\pm)^* \mathbf{N}_s \otimes (\mathbf{F}^\pm)^* \mathbf{N}_s) (\mathbf{F}^\pm)^* \hat{\boldsymbol{\nu}}) dL \\
&= j_A (\mathbf{1} - \mathbf{n}_s \otimes \mathbf{n}_s) (\mathbf{F}^\pm)^{-T} \hat{\boldsymbol{\nu}} dL.
\end{aligned} \tag{6.42}$$

Therefore the Piola stress tensor for surface is given by,

$$\mathbf{P} = j_A \text{TP}_{(\mathbf{n}_s)} (\mathbf{F}^\pm)^{-T}. \tag{6.43}$$

The net dissipation can be written as,

$$D \doteq \int_{\partial\Omega} \mathbf{P} \mathbf{N} \cdot \mathbf{v} dA + \int_{\partial S} \mathbf{P} \hat{\boldsymbol{\nu}} \cdot \mathbf{w} dL - \frac{d}{dt} \int_{\Omega} \Psi dV - \frac{d}{dt} \int_S \phi dA \geq 0, \tag{6.44}$$

where  $\mathbf{w}$  is the edge velocity. Use the surface divergence theorem and the surface transport theorem (cf. (2.105) and (2.117)) to get:

$$\oint_{\partial S} \mathbf{P}^T \mathbf{w} \cdot \hat{\boldsymbol{\nu}} dL = \int_S (\text{Div}^S (\mathbf{P}^T \mathbf{w}) + 2H \mathbf{P} \mathbf{N} \cdot \mathbf{w}) dA, \tag{6.45}$$

and

$$\frac{d}{dt} \int_S \phi dA = \int_S (\overset{\circ}{\phi} - 2\phi UH) dA, \tag{6.46}$$

where  $\text{Div}^S$  and  $(\overset{\circ}{\cdot})$  denotes the surface divergence and the normal time derivative, respectively (cf. Subsection 2.1.4). These relations when substituted into (6.44) will yield (on using localization theorem) the inequality (6.36) in the bulk and also a modified (in comparison to (6.37)) inequality on the interface. The final inequality will require us to calculate  $\overset{\circ}{\phi}$ , which we will illustrate below, for specific constitutive assumptions.

We introduce the following constitutive assumptions regarding the energy densities:

$$\Psi = J_K^{-1} W(\mathbf{H}) + \frac{1}{2} \rho_\kappa \mathbf{v} \cdot \mathbf{v} \quad (6.47)$$

for the bulk and

$$\phi = \mathcal{A}_1 w(\mathbf{H}_1 \mathbb{P}_1, \mathbf{H}_2 \mathbb{P}_2) \quad (6.48)$$

for the interface (see Remark 6.2.1 below). We assume that the interface has a vanishing mass and therefore has no associated inertial terms. Here  $w$  represents the interface energy per unit area of surface 1 in the intermediate configuration (the area element in the reference configuration is mapped into two area elements in the intermediate configuration, which we label as 1 and 2. This is same as using signs  $\pm$ , but provides a more clear notation for the following calculation). In the above  $\mathcal{A}_1$  represents the change in intermediate interface area 1 for every unit change in reference interface area. The projections  $\mathbb{P}_a$  ( $a = 1, 2$ ) are given by  $\mathbb{P}_a = \mathbf{1}_a - \mathbf{n}_a \otimes \mathbf{n}_a$ . Here  $\mathbf{1}_a$  denotes the identity transformation in the intermediate configuration  $a$  and  $\mathbf{n}_a$  as the normals in the intermediate configuration (both of which map to  $\mathbf{n}_s$  in the current configuration and to  $\mathbf{N}_s$  in the reference configuration). Using Nanson's formula we evaluate,  $\mathbf{N}_s dA = J_{K_1} \mathbf{K}_1^{-T} \mathbf{n}_1 dA_1$ . Therefore,

$$\mathcal{A}_1 \equiv \frac{dA_1}{dA} = J_{K_1}^{-1} (\mathbf{K}_1^{-T} \mathbf{n}_1 \cdot \mathbf{N}_s)^{-1}. \quad (6.49)$$

We now calculate  $\dot{\phi}$ . Using (6.48) we write,

$$\dot{\phi} = \dot{\mathcal{A}}_1 w(\mathbf{H}_1 \mathbb{P}_1, \mathbf{H}_2 \mathbb{P}_2) + \mathcal{A}_1 \dot{w}(\mathbf{H}_1 \mathbb{P}_1, \mathbf{H}_2 \mathbb{P}_2), \quad (6.50)$$

where (using (6.49))

$$\begin{aligned}\dot{\mathcal{A}}_1 &= -\mathcal{A}_1 \mathbf{K}_1^{-T} \cdot \dot{\mathbf{K}}_1 - J_{K_1} \mathcal{A}_1^2 (-\mathbf{K}_1^{-T} \dot{\mathbf{K}}_1^T \mathbf{K}_1^{-T} \mathbf{n}_1 \cdot \mathbf{N}_s + \mathbf{K}_1^{-T} \dot{\mathbf{n}}_1 \cdot \mathbf{N}_s + \mathbf{K}_1^{-T} \mathbf{n}_1 \cdot \dot{\mathbf{N}}_s) \\ &= -\mathcal{A}_1 \mathbf{K}_1^{-T} \dot{\mathbf{K}}_1^T \cdot (\mathbf{1} - \mathbf{N}_s \otimes \mathbf{N}_s) - J_{K_1} \mathcal{A}_1^2 \mathbf{K}_1^{-1} \mathbf{N}_s \cdot \dot{\mathbf{n}}_1 - J_{K_1} \mathcal{A}_1^2 \mathbf{K}_1^{-T} \mathbf{n}_1 \cdot \dot{\mathbf{N}}_s.\end{aligned}\quad (6.51)$$

Also

$$\dot{w} = w_{\mathbf{H}_1 \mathbb{P}_1} \cdot (\mathbf{H}_1 \dot{\mathbb{P}}_1) + w_{\mathbf{H}_2 \mathbb{P}_2} \cdot (\mathbf{H}_2 \dot{\mathbb{P}}_2).\quad (6.52)$$

Since  $\mathbf{H}_a \dot{\mathbb{P}}_a = \dot{\mathbf{F}}_a \mathbf{K}_a \mathbb{P}_a + \mathbf{F}_a \mathbf{K}_a \dot{\mathbb{P}}_a$  (no summation over  $a$ ), we obtain

$$\begin{aligned}\dot{w} &= w_{\mathbf{H}_1 \mathbb{P}_1} \cdot (\dot{\mathbf{F}}_1 \mathbf{K}_1 \mathbb{P}_1 + \mathbf{F}_1 \mathbf{K}_1 \dot{\mathbb{P}}_1) + w_{\mathbf{H}_2 \mathbb{P}_2} \cdot (\dot{\mathbf{F}}_2 \mathbf{K}_2 \mathbb{P}_2 + \mathbf{F}_2 \mathbf{K}_2 \dot{\mathbb{P}}_2) \\ &= \sum_{a=1}^2 (w_{\mathbf{H}_a \mathbb{P}_a} \mathbb{P}_a \mathbf{K}_a^T \cdot \dot{\mathbf{F}}_a) + \sum_{a=1}^2 (\mathbf{F}_a^T w_{\mathbf{H}_a \mathbb{P}_a} \cdot \mathbf{K}_a \dot{\mathbb{P}}_a).\end{aligned}\quad (6.53)$$

*Remark 6.2.1.* (Surface energy density) The atomic configuration near the interface is significantly different from that in the bulk [17]. The energetic response to the distortion of the underlying lattice will, therefore, also differ from the bulk energy responses. The interfacial energy, as we shall show below, depends not only on the strain values, but also on the relative orientation of the intersecting lattices. Following Gibbs, we define the surface energy density  $\phi$  (surface energy per unit area of the interface in the reference configuration) by

$$E = \int_{\Omega} \Psi dV + \int_S \phi dA,\quad (6.54)$$

where  $E$  is the total energy associated with  $\Omega \in \kappa_i$  such that  $S = \Omega \cap S_t \neq \emptyset$ . Therefore, the interface energy can be seen as the excess energy contribution to an otherwise bulk energy.

The surface energy density  $\phi$  is related to the  $w$ , which is the surface energy per unit area of surface 1 in the intermediate configuration, by  $\phi = \mathcal{A}_1 w$ , where  $\mathcal{A}_1$  is defined in (6.49).

Start by assuming  $w$  to be a function of  $\mathbf{K}_a$  and  $\mathbf{H}_a$  ( $a = 1, 2$ ). But using the result from

Section 6.1, we note that a dependence of  $w$  on  $\mathbf{K}_a$  can only be through the true surface dislocation density tensors. However, the true surface dislocation density tensors can also be expressed in terms of  $\mathbf{H}_a$  (cf. (5.44)), and thus the constitutive function  $w$  can be expressed as a function of  $\mathbf{H}_a$ . Note that to reach this conclusion, we have only used the invariance of  $w$  with respect to compatible changes in the reference configuration. We next assume that the energy  $w$  is insensitive to any out of plane (of the interface) lattice distortion. This implies that  $w$  is independent of the normal components of  $\mathbf{H}_a$ , i.e. of  $\mathbf{H}_a \mathbf{n}_a$ . The roots of this assumption lies in our work postulate, where we assume surface stress to do work in association with the edge velocity (which lies in the plane of the interface). This combined with our constitutive assumption regarding stress implies that there is no mechanism to store surface energy corresponding to the normal components of  $\mathbf{H}_a$  (Cermelli & Gurtin [29] proved this result using the dissipation inequality, but in a slightly different context than discussed here). We therefore have the interface energy with functional dependence as mentioned in (6.48).

Further, subject  $w$  to the invariance with respect to superimposed rigid body motions. Use the polar decomposition  $\mathbf{H}_a = \mathbf{R}_a \mathbf{U}_a$ , where  $\mathbf{R}_a \in Orth^+$  and  $\mathbf{U}_a \in Sym^+$ . Under a superimposed rigid body motion, denoted by  $\mathbf{Q} \in Orth$ ,  $\mathbf{H}_a$  transforms to  $\mathbf{Q} \mathbf{H}_a$ . Choose  $\mathbf{Q} = \mathbf{R}_1^T$ . We then obtain the following necessary condition for  $w$  to be invariant:

$$w = \hat{w}(\mathbf{U}_1 \mathbb{P}_1, \mathbf{R} \mathbf{U}_2 \mathbb{P}_2), \quad (6.55)$$

where  $\mathbf{R} \in Orth^+$  denotes the relative rotation of material points across the interface. Moreover,  $w$  should be insensitive to the normal components  $\mathbf{U}_a \mathbf{n}_a$ , since otherwise our assumption of the insensitivity (of  $w$ ) to the out-of-plane deformation will be violated.

Noting that  $\mathbf{U}_a$  are symmetric, we should have the following form for  $w$ :

$$w = \check{w}(\mathbb{P}_1 \mathbf{U}_1 \mathbb{P}_1, \mathbf{R} \mathbb{P}_2 \mathbf{U}_2 \mathbb{P}_2). \quad (6.56)$$

Define  $C_a = \mathbb{P}_a \mathbf{C}_a \mathbb{P}_a$ , where  $\mathbf{C}_a = \mathbf{U}_a^2$ . Using the identity  $\mathbb{P}_a^2 = \mathbb{P}_a$  we can therefore obtain from (6.56)

$$w = \bar{w}(C_a, \mathbf{R}). \quad (6.57)$$

If  $\mathbf{C}_a = \mathbf{1}_a$ , i.e. the bulk on either side of the interface is unstrained, then the representation (6.57) reduces to

$$w = \bar{w}(\mathbb{P}_a, \mathbf{R}). \quad (6.58)$$

In the unstrained case, therefore, the surface energy is a function of normals at the interface and the relative rotation. Such energies are widely studied in the literature on metal interfaces, in particular grain boundaries, and many experimental methods have been determined for their evaluation (see for example the article by Herring in [58] and the books by Howe [77] and Gottstein & Shvindlerman [59]).

In much of the classical literature on surface/interface science, the free energy per unit area of the interface in the current configuration is also called surface tension (per unit length in the surface) [23, 155, 137]. This equivalence is motivated from the studies of liquid surfaces, and surface tension should not be confused with surface stress.

# Bibliography

- [1] A. Acharya. A model of crystal plasticity based on the theory of continuously distributed dislocations. *Journal of Mechanics and Physics of Solids*, 49:761–784, 2001.
- [2] A. Acharya and J. L. Bassani. Lattice incompatibility and a gradient theory of crystal plasticity. *Journal of Mechanics and Physics of Solids*, 48:1562–1595, 2000.
- [3] S. Amelinckx. *The Direct Observation of Dislocations*. Academic Press, New York and London, 1964.
- [4] A. S. Argon. *Strengthening Mechanisms in Crystal Plasticity*. Oxford University Press, 2008.
- [5] A. Arsenlis and D. M. Parks. Crystallographic aspects of geometrically–necessary and statistically–stored dislocation density. *Acta Materialia*, 47(5):1597–1611, 1999.
- [6] M. F. Ashby. The deformation of plastically non–homogeneous materials. *Philosophical Magazine*, 21:399–424, 1970.
- [7] M. M. Balaban, A. E. Green, and P. M. Naghdi. Acceleration waves in elastic–plastic materials. 8:315–335, 1970.

- [8] J. M. Ball and R. D. James. Proposed experimental tests of a theory of fine microstructure and the two-well problem. *Philosophical Transactions of the Royal Society of London A*, 338:389–450, 1992.
- [9] Z. S. Basinski and J. W. Christian. Interpenetrating bands in transformed indium–thallium alloys. *Acta Metallurgica*, 4:371–378, 1956.
- [10] F. Basson and J. H. Driver. Modelling the evolution of geometrically necessary boundaries at large plastic strains. *Materials Science and Engineering A*, 256:243–255, 1998.
- [11] J. F. Bell. The decrease of volume during loading to finite plastic strain. *Meccanica*, 31:461–472, 1996.
- [12] B. A. Bilby. Types of dislocation source. In *Report of Bristol Conference on Defects in Crystalline Solids*, pages 124–133. London: Physical Society, 1955.
- [13] B. A. Bilby, R. M. Bullough, and D. K. de Grinberg. General theory of surface dislocations. *Discussions of the Faraday Society*, 38:61–68, 1964.
- [14] B. A. Bilby, R. M. Bullough, and E. Smith. Continuous distributions of dislocations: a new application of the methods of non-Riemannian geometry. *Proceedings of the Royal Society at London A*, 231:263–273, 1955.
- [15] Ph. Boulanger and M. Hayes. Bounds on elastic wave speeds in crystals: Theory and applications. *Proceedings of the Royal Society at London A*, 454:2289–2322, 1998.
- [16] W. L. Bragg. Discussion to ‘Geometrical considerations concerning the structural

- irregularities to be assumed in a crystal'. *Proceedings of the Physical Society*, 52:54–55, 1940.
- [17] R. M. Brick, editor. *Metal Interfaces*. American Society of Metals, Cleveland, Ohio, 1953. Proceedings of the seminar on metal interfaces held during the thirty-third national metal congress and exposition, Detroit, October 13 to 19, 1951, sponsored by the American Society for Metals.
- [18] P. W. Bridgman. *The Nature of Thermodynamics*. Harvard University Press, 1943.
- [19] P. W. Bridgman. Volume changes in the plastic stages of simple compression. *Journal of Applied Physics*, 20:1241–1251, 1949.
- [20] P. W. Bridgman. The thermodynamics of plastic deformation and generalized entropy. *Review of Modern Physics*, 22(1):56–63, 1950.
- [21] P. W. Bridgman. Reflections on thermodynamics. *American Scientist*, 41(4):549–555, 1953. Reprinted as an appendix to the revised edition of [18].
- [22] P. W. Bridgman. *Studies in Large Plastic Flow and Fracture*. Harvard University Press, 1964.
- [23] R. C. Brown. The fundamental concepts concerning surface tension and capillarity. *Proceedings of the Physical Society*, 59:429–448, 1947.
- [24] V. Bulatov and W. Cai. *Computer Simulations of Dislocations*. Oxford University Press, 2006.



- [25] R. M. Bullough and B. A. Bilby. Continuous distributions of dislocations: surface dislocations and the crystallography of martensitic transformations. *Proceedings of the Physical Society B*, 69:1276–1286, 1956.
- [26] J. M. Burgers. Geometrical considerations concerning the structural irregularities to be assumed in a crystal. *Proceedings of the Physical Society*, 52:23–33, 1940.
- [27] J. D. Campbell. *Dynamic Plasticity of Metals*. Springer–Verlag, 1970. Courses and Lectures – No. 46, International Centre for Mechanical Sciences, Udine.
- [28] O. Cazacu and F. Barlat. Application of the theory of representation to describe yielding of anisotropic aluminum alloys. *International Journal of Engineering Science*, 41:1367–1385, 2003.
- [29] P. Cermelli and M. E. Gurtin. The dynamics of solid–solid phase transitions 2. Incoherent interfaces. *Archive of Rational Mechanics and Analysis*, 127:41–99, 1994.
- [30] P. Cermelli and M. E. Gurtin. On the characterization of geometrically necessary dislocations in finite plasticity. *Journal of Mechanics and Physics of Solids*, 49:1539–1568, 2001.
- [31] P. Cermelli and S. Sellers. Multi–phase equilibrium of crystalline solids. *Journal of Mechanics and Physics of Solids*, 48:765–796, 2000.
- [32] P. Chadwick. *Continuum Mechanics: Concise Theory and Problems*. Dover, 1999.
- [33] H. Chang. *Inventing Temperature: Measurement and Scientific Progress*. Oxford University Press, 2004.

- [34] P. J. Chen. Growth and decay of waves in solids. In S. Flügge, editor, *Handbuch der Physik*, volume VIa/3, pages 303–402. Springer–Verlag, 1973.
- [35] J. W. Christian. *The Theory of Transformations in Metals and Alloys (Part I)*, 3rd Edition. Pergamon, 2002.
- [36] J. W. Christian and S. Mahajan. Deformation twinning. *Progress in Materials Science*, 39:1–157, 1995.
- [37] H. Cohen and M. Epstein. Remarks on uniformity in hyperelastic materials. *International Journal of Solids and Structures*, 20(3):233–243, 1984.
- [38] A. H. Cottrell. *Dislocations and Plastic Flow in Crystals*. Oxford University Press, 1958.
- [39] R. Courant and K. O. Friedrichs. *Supersonic Flow and Shock Waves*. Interscience Publishers, Inc., New York, 1948.
- [40] J. W. Craggs. The propagation of infinitesimal plane waves in elastic–plastic materials. *Journal of Mechanics and Physics of Solids*, 5:115–124, 1957.
- [41] R. M. Davies. Stress waves in solids. In G. K. Batchelor and R. M. Davies, editors, *Surveys in Mechanics*, pages 64–161. Cambridge University Press, 1956.
- [42] C. Davini. Elastic invariants in crystal theory. In J. M. Ball, editor, *Material Instabilities in Continuum Mechanics and Related Mathematical Problems*, pages 85–105. Oxford, 1988.

- [43] D. C. Drucker. Some implications of work hardening and ideal plasticity. *Quarterly of Applied Mathematics*, 7:411–418, 1950.
- [44] C. Eckart. The thermodynamics of irreversible processes. IV: The theory of elasticity and anelasticity. *Physical Review*, 73:373–382, 1948.
- [45] M. Epstein. Toward a complete second order evolution law. *Mathematics and Mechanics of Solids*, 4(2):251–266, 1999.
- [46] M. Epstein. Self-driven continuous dislocations and growth. In P. Steinmann and G. A. Maugin, editors, *Mechanics of Material Forces*, pages 129–139. Springer, Berlin, 2005.
- [47] M. Epstein and G. A. Maugin. The energy–momentum tensor and material uniformity in finite elasticity. *Acta Mechanica*, 83:127–133, 1990.
- [48] M. Epstein and G. A. Maugin. On the geometrical material structure of anelasticity. *Acta Mechanica*, 115:119–131, 1996.
- [49] J. L. Ericksen. Special topics in elastostatics. *Advances in Applied Mechanics*, 17:189–244, 1977.
- [50] F. I. Fedorov. *Theory of Elastic Waves in Crystals*. Plenum Press, New York, 1968.
- [51] F. D. Fischer, T. Waitz, D. Vollath, and N. K. Simha. On the role of surface energy and surface stress in phase-transforming nanoparticles. *Progress in Materials Science*, 53:481–527, 2008.

- [52] N. A. Fleck, G. M. Muller, M. F. Ashby, and J. W. Hutchinson. Strain gradient plasticity: theory and experiments. *Acta Metallurgica Materialia*, 42:475–487, 1994.
- [53] R. Fosdick and H. Tang. Surface transport in continuum mechanics. *Mathematics and Mechanics of Solids*, In Press, 2008.
- [54] F. C. Frank. The resultant content of dislocations in an arbitrary intercrystalline boundary. In *A Symposium on the Plastic Deformation of Crystalline Solids, Mellon Institute, Pittsburgh, 19, 20 May 1950, under the joint sponsorship of the Carnegie Institute of Technology and the Department of the Navy, Office of Naval Research*, pages 150–154. Washington : U.S. Government Printing Office, 1950.
- [55] E. Fried and M. E. Gurtin. A unified treatment of evolving interfaces accounting for deformation and atomic transport with an emphasis on grain-boundaries and epitaxy. *Advances in Applied Mechanics*, 40:1–177, 2004.
- [56] P. Germain and E. H. Lee. On shock waves in elastic–plastic solids. *Journal of Mechanics and Physics of Solids*, 21:359–382, 1973.
- [57] P. Glansdorff and I. Prigogine. *Thermodynamic Theory of Structure, Stability and Fluctuations*. Wiley–Interscience, 1971.
- [58] R. Gomer and C S Smith, editors. *Structure and Properties of Solid Interfaces*. The University of Chicago Press, 1953. Proceedings of the conference arranged by the National Research Council, Lake Geneva, Wisconsin, September 1952.
- [59] G. Gottstein and L. S. Shvindlerman. *Grain Boundary Migration in Metals: Thermodynamics, Kinetics, Applications*. CRC Press, 1999.

- [60] A. E. Green and J. E. Adkins. *Large Elastic Deformations (2nd edition)*. Oxford University Press, Oxford, 1970.
- [61] A. E. Green and P. M. Naghdi. A thermodynamic development of elastic–plastic continua. In H. Parkus and L. I. Sedov, editors, *Irreversible Aspects of Continuum Mechanics*, pages 117–131. Springer–Verlag, 1968. IUTAM Symposia Vienna, June 22–28, 1966.
- [62] A. E. Green and R. S. Rivlin. On Cauchy’s equations of motion. *Zeitschrift für angewandte Mathematik und Physik*, 15:290–292, 1964.
- [63] W. A. Green. Acceleration waves at an elastic/plastic loading interface. *International Journal of Engineering Science*, 1:523–532, 1970.
- [64] S. R. de Groot and P. Mazur. *Non–equilibrium Thermodynamics*. Dover, 1984.
- [65] A. Gupta and D. J. Steigmann. Kinematics and balance laws. In *Continuum Mechanics: Encyclopedia of Life Support Systems (EOLSS)*, UNESCO. Eolss Publishers, Oxford, UK, 2008.
- [66] A. Gupta, D. J. Steigmann, and J. Stölken. On the evolution of plasticity and incompatibility. *Mathematics and Mechanics of Solids*, 12:583–610, 2007.
- [67] M. E. Gurtin. *An Introduction to Continuum Mechanics*. Academic Press, 1981.
- [68] M. E. Gurtin. A gradient theory of single–crystal viscoplasticity that accounts for geometrically necessary dislocations. *Journal of Mechanics and Physics of Solids*, 50:5–32, 2002.

- [69] M. E. Gurtin and L. Anand. The decomposition  $F = F^e F^p$ , material symmetry, and plastic irrotationality for solids that are isotropic-viscoplastic or amorphous. *International Journal of Plasticity*, 21:1686–1719, 2005.
- [70] M. E. Gurtin and L. Anand. A theory of strain–gradient plasticity for isotropic, plastically irrotational materials. Part I: Small deformations. *Journal of Mechanics and Physics of Solids*, 53:1624–1649, 2005.
- [71] M. E. Gurtin and L. Anand. A theory of strain–gradient plasticity for isotropic, plastically irrotational materials. Part II: Finite deformations. *International Journal of Plasticity*, 21:2297–2318, 2005.
- [72] P. Hähner. On the foundations of stochastic dislocation dynamics. *Applied Physics A*, 62:473–481, 1996.
- [73] R. Hill. Acceleration waves in solids. *Journal of Mechanics and Physics of Solids*, 10:1–16, 1962.
- [74] R. Hill. Aspects of invariance in solid mechanics. *Advances in Applied Mechanics*, 18:1–75, 1978.
- [75] R. Hill. *The Mathematical Theory of Plasticity (Oxford Classic Texts in the Physical Sciences)*. Oxford University Press, 1998.
- [76] J. P. Hirth and J. Lothe. *Theory of Dislocations*. Krieger Publishing Company, 1992.
- [77] J. M. Howe. *Interfaces in Metals: Atomic Structure, Thermodynamics and Kinetics*

- of Solid–Vapor, Solid–Liquid and Solid–Solid Interfaces.* John Wiley & Sons Inc., 1997.
- [78] D. A. Hughes, N. Hansen, and D. J. Bammann. Geometrically necessary boundaries, incidental dislocation boundaries and geometrically necessary dislocations. *Scripta Materialia*, 48:147–153, 2003.
- [79] A. A. Il’iushin. O prirashchenii plasticheskoi deformatsii i poverkhnosti tekuchesti. *Prikladnaya Matematika i Mekhanika*, 24(4):663–666, 1960. English translation: On the increments of plastic deformations and the yield surface. *Journal of Applied Mathematics and Mechanics*, 25(4):987–992, 1960.
- [80] A. A. Il’iushin. O postulate plastichnosti. *Prikladnaya Matematika i Mekhanika*, 25(3):503–507, 1961. English translation: On the postulate of plasticity. *Journal of Applied Mathematics and Mechanics*, 25(3):746–752, 1961.
- [81] J. V. José and E. J. Saletan. *Classical Dynamics: A Contemporary Approach.* Cambridge University Press, 1998.
- [82] L. M. Kachanov. *Fundamentals of the Theory of Plasticity.* Dover, 2004.
- [83] A. Kadić and D. G. B. Edelen. *A Gauge Theory of Dislocations and Disclinations, Lecture Notes in Physics 174.* Springer, 1983.
- [84] J. Kestin. On the application of the principles of thermodynamics to strained solid materials. In H. Parkus and L. I. Sedov, editors, *Irreversible Aspects of Continuum Mechanics*, pages 177–212. Springer–Verlag, 1968. IUTAM Symposia Vienna, June 22–28, 1966.

- [85] J. Kestin. Thermodynamics of plastic deformation. In D. Walgraef, editor, *Patterns, Defects and Microstructures in Non-equilibrium Systems*, pages 202–219. Martinus Nijhoff Publishers, 1987.
- [86] J. Kestin and J. R. Rice. Paradoxes in the application of thermodynamics to strained solids. In E. G. Stuart, B. Gal-Or, and A. J. Brainard, editors, *A Critical Review of Thermodynamics*, pages 275–298. Mono Book Corp., 1970.
- [87] D. Kondepudi and I. Prigogine. *Modern Thermodynamics: From Heat Engines to Dissipative Structures*. John Wiley & Sons Inc., 1998.
- [88] K. Kondo. Non-Riemannian geometry of imperfect crystals from a macroscopic viewpoint. In K. Kondo, editor, *Volume 1 of RAAG Memoirs of the Unifying Study of Basic Problems in Engineering and Physical Science by Means of Geometry*. Gakujutsu Bunken Fukyu-Kai, Tokyo, 1955.
- [89] A. M. Kosevich. The deformation field in an isotropic elastic medium containing moving dislocations. *Soviet Physics JETP*, 15(1):108–115, 1965.
- [90] A. M. Kosevich. Dynamical theory of dislocations. *Soviet Physics Uspekhi*, 7(6):837–854, 1965.
- [91] E. Kröner. Allgemeine kontinuumstheorie der versetzungen und eigenspannungen. *Archive of Rational Mechanics and Analysis*, 4:273–334, 1960.
- [92] E. Kröner. Initial studies of a plasticity theory based upon statistical mechanics. In M. F. Kanninen et al., editor, *Inelastic Behavior of Solids*, pages 137–148. McGraw-Hill Book Company, 1970.



- [93] E. Kröner. Continuum theory of defects. In R. Balian et al., editor, *Les Houches, Session XXXV, 1980 – Physique des défauts*, pages 215–315. North-Holland, New York, 1981.
- [94] I. A. Kunin. Fields of randomly distributed dislocations and force dipoles in an infinite elastic anisotropic medium. *Zhurnal Prikladnoi Mekhaniki Tekhnicheskoi Fiziki*, 5:76–83, 1965.
- [95] I. A. Kunin. *Elastic Media with Microstructure II*. Springer–Verlag, 1983.
- [96] L. D. Landau and E. M. Lifshitz. *Theory of Elasticity, 3rd Edition: (Course of Theoretical Physics, Vol. 7)*. Butterworth–Heinemann, 1986.
- [97] F. C. Larché and J. W. Cahn. Thermomechanical equilibrium of multi–phase solids under stress. *Acta Materialia*, 26:1579–1589, 1978.
- [98] F. C. Larché and J. W. Cahn. The interaction of composition and stress in crystalline solids. *Acta Materialia*, 33:331–357, 1985.
- [99] R. W. Lardner. *Mathematical Theory of Dislocations and Fracture*. University of Toronto Press, Toronto, 1974.
- [100] B. C. Larson, A. El-Azab, and W. Yang et al. Experimental characterization of the mesoscale dislocation density tensor. *Philosophical Magazine*, 87:1327–1347, 2007.
- [101] P. D. Lax. Development of singularities of solutions of nonlinear hyperbolic partial differential equations. *Journal of Mathematical Physics*, 5:611–613, 1964.

- [102] P. D. Lax. Hyperbolic systems of conservation laws and the mathematical theory of shock waves. In *Regional Conference Series in Applied Mathematics*, pages 1–48. SIAM, Philadelphia, 1973.
- [103] E. H. Lee. Elastic plastic deformation at finite strain. *ASME Journal of Applied Mechanics*, 36:1–6, 1969.
- [104] J. M. Lee. *Introduction to Smooth Manifolds*. Springer, 2003.
- [105] P. H. Leo and R. F. Sekerka. The effect of surface stress on crystal–melt and crystal–crystal equilibrium. *Acta Materialia*, 37:3119–3138, 1989.
- [106] C. H. Li, E. H. Edwards, J. Washburn, and E. R. Parker. Stress–induced movement of crystal boundaries. *Acta Metallurgica*, 1:223–229, 1953.
- [107] J. Lubliner. Acceleration waves in generalized elastic–plastic continua. *Acta Mechanica*, 58:193–200, 1986.
- [108] J. Lubliner. Normality rules in large–deformation plasticity. *Mechanics of Materials*, 5:29–34, 1986.
- [109] J. Lubliner. *Plasticity Theory (revised edition)*. Available online with the permission of author, 2006. An earlier version of this book was published in 1990 by Pearson Education, Inc.
- [110] M. Lucchesi and P. Podio-Guidugli. Equivalent dissipation postulates in classical plasticity. *Meccanica*, 25:26–31, 1990.

- [111] M. Lucchesi and P. Podio-Guidugli. Materials with elastic range: A theory with a view towards applications. Part II. *Archive of Rational Mechanics and Analysis*, 110:9–42, 1990.
- [112] M. Lucchesi and M. Šilhavý. Il'yushin's conditions in non-isothermal plasticity. *Archive of Rational Mechanics and Analysis*, 113:121–163, 1991.
- [113] C. S. Man, X. Gao, S. Godefroy, and E. A. Kenik. Estimating geometric dislocation densities in polycrystalline materials from orientation imaging microscopy. *Preprint*, 2008.
- [114] J. Mandel. Ondes plastiques dans un milieu indéfini à trois dimensions. *Journal de Mécanique*, 1:3–30, 1962.
- [115] J. Mandel. Equations constitutives et directeurs dans les milieux plastiques et viscoplastiques. *International Journal of Solids and Structures*, 9:725–740, 1973.
- [116] X. Markenscoff and A. Gupta, editors. *Collected Works of J. D. Eshelby: The Mechanics of Defects and Inhomogeneities (Solid Mechanics and Its Applications)*. Springer, 2006.
- [117] M. A. Meyers. *Dynamic Behavior of Materials*. John Wiley & Sons Inc., 1994.
- [118] N. F. Mott. Dislocations in crystalline solids. In G. K. Batchelor and R. M. Davies, editors, *Surveys in Mechanics*, pages 32–63. Cambridge University Press, 1956.
- [119] H. Mughrabi. On the current understanding of strain gradient plasticity. *Materials Science and Engineering A*, 387389:209–213, 2004.

- [120] T. Mura. On dynamic problems of continuous distribution of dislocations. *International Journal of Engineering Science*, 1:371–381, 1963.
- [121] M. J. P. Musgrave. *Crystal Acoustics*. Holden–Day, San Francisco, 1970.
- [122] F. R. N. Nabarro. *Theory of Crystal Dislocations*. Dover, 1987.
- [123] F. R. N. Nabarro and M. S. Duesbery, editors. *Dislocations in Solids, Volume 11*. Elsevier, 2002.
- [124] P. M. Naghdi. A critical review of the state of finite plasticity. *Zeitschrift für angewandte Mathematik und Physik*, 41:315–394, 1990.
- [125] P. M. Naghdi and A. R. Srinivasa. A dynamical theory of structured solids: I. Basic development. *Philosophical Transactions of the Royal Society of London A*, 345:425–458, 1993.
- [126] P. M. Naghdi and J. A. Trapp. The significance of formulating plasticity theory with reference to loading surfaces in strain space. *International Journal of Engineering Science*, 13:785–797, 1975.
- [127] W. D. Nix and H. Gao. Indentation size effects in crystalline materials: a law for strain gradient plasticity. *Journal of Mechanics and Physics of Solids*, 46:411–425, 1998.
- [128] W. Noll. A mathematical theory of the mechanical behavior of continuous media. *Archive of Rational Mechanics and Analysis*, 2:197–226, 1958.

- [129] W. Noll. Materially uniform simple bodies with inhomogeneities. *Archive of Rational Mechanics and Analysis*, 27:1–32, 1967.
- [130] W. Noll. A new mathematical theory of simple materials. *Archive of Rational Mechanics and Analysis*, 48:1–50, 1972.
- [131] W. Noll. *Foundations of Mechanics and Thermodynamics: Selected Papers*. Springer–Verlag, 1974.
- [132] W. K. Nowacki. *Stress Waves in Non-elastic Solids*. Pergamon, 1978.
- [133] J. W. Nunziato and W. Herrmann. The general theory of shock waves in elastic nonconductors. *Archive of Rational Mechanics and Analysis*, 47:272–287, 1972.
- [134] J. F. Nye. Some geometrical relations in dislocated crystals. *Acta Metallurgica*, 1(2):153–162, 1953.
- [135] G. B. Olson and M. Cohen. Interphase–boundary dislocations and the concept of coherency. *Acta Materialia*, 27:1907–1918, 1979.
- [136] E. Orowan. Zur kristallplastizität: Parts I, II, and III. *Zeitschrift für Physik A Hadrons and Nuclei*, 89:605–659, 1934.
- [137] E. Orowan. Surface energy and surface tension in solids and liquids. *Proceedings of the Royal Society at London A*, 316:473–491, 1970.
- [138] G. P. Parry. Generalized elastic–plastic decompositions in defective crystals. In G. Capriz and P. M. Mariano, editors, *Advances in Multifield Theories for Continua with Substructure*, pages 33–50. Birkhäuser, 2004.

- [139] G. P. Parry and M. Šilhavý. Elastic invariants in the theory of defective crystals. *Proceedings of the Royal Society at London A*, 455:4333–4346, 1999.
- [140] P. Perzyna. Fundamental problems in viscoplasticity. *Advances in Applied Mechanics*, 9:243–377, 1966.
- [141] P. Perzyna. Thermodynamic theory of viscoplasticity. *Advances in Applied Mechanics*, 11:313–354, 1971.
- [142] A. B. Pippard. *The Elements Of Classical Thermodynamics*. Cambridge University Press, 1961.
- [143] M. Pitteri. Reconciliation of local and global symmetries of crystals. *Journal of Elasticity*, 14:175–190, 1984.
- [144] M. Polanyi. Über eine art gitterstörung, die einen kristall plastisch machen könnte. *Zeitschrift für Physik A Hadrons and Nuclei*, 89:660–664, 1934.
- [145] W. Prager and P. G. Hodge. *Theory of Perfectly Plastic Solids*. John Wiley & Sons Inc., 1965.
- [146] I. Prigogine. *Introduction to Thermodynamics of Irreversible Processes*. John Wiley & Sons Inc., 1968.
- [147] K. R. Rajagopal and A. R. Srinivasa. Inelastic behavior of materials. Part I: Theoretical underpinnings. *International Journal of Plasticity*, 14:945–967, 1998.
- [148] K. R. Rajagopal and A. S. Wineman. A constitutive equation for non-linear elastic

- materials which undergo deformation induced microstructural changes. *International Journal of Plasticity*, 8:385–395, 1992.
- [149] W. T. Read and W. Shockley. Dislocation models of crystal grain boundaries. *Physical Review*, 78(3):275–289, 1950.
- [150] W. D. Robertson and N. A. Gjostein, editors. *Metal Surfaces: Structure, Energetics and Kinetics*. American Society of Metals, Metals Park, Ohio, 1963. Papers presented at a joint seminar of the American Society for Metals and the Metallurgical Society of AIME, October 27 and 28, 1962.
- [151] R. T. Rockafellar. *Convex Analysis (Princeton Landmarks in Mathematics and Physics)*. Princeton University Press, 1996.
- [152] W. Rudin. *Principles of Mathematical Analysis*. McGraw–Hill, 1976.
- [153] F. Schuricht. A new mathematical foundation for contact interactions in continuum physics. *Archive of Rational Mechanics and Analysis*, 184(3):495–551, 2007.
- [154] J. Serrin, editor. *New Perspectives in Thermodynamics*. Springer–Verlag, 1986.
- [155] R. Shuttleworth. The surface tension of solids. *Proceedings of the Physical Society A*, 63:444–457, 1950.
- [156] M. Šilhavý. *The Mechanics and Thermodynamics of Continuous Media (Texts and Monographs in Physics)*. Springer, 1997.
- [157] M. Šilhavý. Work conditions and energy functions for ideal elastic–plastic materials.

- In G. Capriz and P. M. Mariano, editors, *Advances in Multifield Theories for Continua with Substructure*, pages 1–31. Birkhäuser, 2004.
- [158] C. S. Smith. Metallographic studies of metals after explosive shock. *Transactions of the Metallurgical Society of AIME*, 212:574–589, 1958.
- [159] C. S. Smith. *A Search for Structure: Selected Essays on Science, Art, and History*. MIT Press, 1982.
- [160] J. S. Stölken and A. G. Evans. A microbend test method for measuring the plasticity length scale. *Acta Materialia*, 46:5109–5115, 1998.
- [161] A. P. Sutton and R. W. Balluffi. *Interfaces in Crystalline Materials (Monographs on the Physics and Chemistry of Materials)*. Oxford University Press, 2007.
- [162] G. I. Taylor. The mechanism of plastic deformation of crystals. Part I: Theoretical, Part II: Comparison with observations. *Proceedings of the Royal Society at London A*, 145:362–404, 1934.
- [163] G. I. Taylor. The testing of materials at high strain rates of loading. *Journal of the Institution of Civil Engineers*, 8:486–519, 1946.
- [164] C. Teodosiu. *Elastic Models of Crystal Defects*. Springer-Verlag, 1982.
- [165] T. Y. Thomas. *Plastic Flow and Fracture in Solids*. Academic Press, 1961.
- [166] S. Cleja-Țigoiu. Models in multiplicative finite elasto-plasticity. In G. A. Maugin, editor, *Geometry, Continua and Microstructure*, pages 75–85. Hermann, paris, 1999.



- [167] S. Cleja-Țigoiu. Dissipative nature of plastic deformations in finite anisotropic elastoplasticity. *Mathematics and Mechanics of Solids*, 8:575–613, 2003.
- [168] S. Cleja-Țigoiu and E. Soos. Elastoviscoplastic models with relaxed configurations and internal state variables. *Applied Mechanics Review*, 43(7):131–151, 1990.
- [169] C. Truesdell, editor. *Rational Thermodynamics*. Springer-Verlag, 1984.
- [170] C. Truesdell and W. Noll. *The Non-Linear Field Theories of Mechanics, Third Edition*. Springer, 2004.
- [171] C. Truesdell and R. A. Toupin. The classical field theories. In S. Flügge, editor, *Handbuch der Physik*, volume III/1, pages 226–793. Springer-Verlag, 1960.
- [172] C. C. Wang. On the geometric structures of simple bodies, a mathematical foundation for the theory of continuous distribution of dislocations. *Archive of Rational Mechanics and Analysis*, 27:33–94, 1967.
- [173] J. Weertman. Plastic deformation behind strong shock waves. *Mechanics of Materials*, 5:13–28, 1986.
- [174] J. Weertman and J. R. Weertman. *Elementary Dislocation Theory*. Oxford University Press, 1992.
- [175] H. Weyl. Shock waves in arbitrary fluids. *Communications on Pure and Applied Mathematics*, 2:103–122, 1949.
- [176] J. R. Willis. Second-order effects of dislocations in anisotropic crystals. *International Journal of Engineering Science*, 5:171–190, 1967.

- [177] A. S. Wineman and K. R. Rajagopal. On a constitutive theory for materials undergoing microstructural changes. *Archives of Mechanics*, 42:53–74, 1990.
- [178] Q. S. Zheng. Theory of representations for tensor functions: A unified invariant approach to constitutive equations. *Applied Mechanics Review*, 47:545–587, 1994.