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On Structured Surfaces with Defects: Geometry, Strain Incompatibility, Stress Field, and Natural Shapes

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Abstract Given a distribution of defects on a structured surface, such as those represented by 2-dimensional crystalline materials, liquid crystalline surfaces, and thin sandwiched shells, what is the resulting stress field and the deformed shape? Motivated by this concern, we first classify, and quantify, the translational, rotational, and metrical defects allowable over a broad class of structured surfaces. With an appropriate notion of strain, the defect densities are then shown to appear as sources of strain incompatibility. The strain incompatibility relations, aided with a decomposition of strain into elastic and plastic parts, and the stress equilibrium relations, with a suitable choice of material response, provide the necessary equations for determining both the stress field and the deformed shape. We demonstrate this by applying our theory to Kirchhoff–Love shells with a kinematics which allows for small surface strains but moderately large rotations. We discuss implications of our framework in the context of 2-dimensional crystals, growing biological membranes, and isotropic fluid films.

Keywords 2-Dimensional materials · Thin structures · Geometry of defects · Surface dislocations · Surface disclinations · Non-metricity · Strain incompatibility · 2-Dimensional crystals · Biological growth · Fluid films

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1 Introduction

The aim of this article is to study geometry and mechanics of defects in structured surfaces. The term *structured surface* is used to represent a variety of 2-dimensional material surfaces such as 2-dimensional crystals (colloidosomes, carbon nanotubes, graphene, etc.); thin sandwiched structures; liquid crystalline membranes and shells, with intrinsic crystalline order

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(single-layer viral capsids) or without (nematic membranes, single layers in smectics and cholesterics); and Cosserat surfaces, which are used to model a hierarchy of plate and shell theories for thin elastic structures abundant in structural and biomechanical applications. The defects are anomalies within the local arrangement of entities in an ordered structure, where the order is usually defined in terms of translational, rotational, and metrical symmetries of the underlying material. These anomalies are omnipresent in nature, e.g., edge dislocations (translational anomalies), wedge disclinations (rotational anomalies), and point imperfections (metric anomalies) such as vacancies and self-interstitials in 2-dimensional crystalline membranes [8, 51]; twist and wedge disclinations, and edge and screw dislocations in liquid crystalline surfaces [32, 33]; see Sect. 2 for more examples. We also include the phenomena of thermal deformation and biological growth as those leading to metric anomalies since they bring about metrical changes in the material space [4, 60]. Defects can also appear as global anomalies which affect the topology of the surface, such as those present in multiply connected and non-orientable surfaces [8, 26, 27, 57, 58]. Many of the superior physicochemical properties of the 2-dimensional defective structures can be attributed to the stress fields resulting from the distribution of defects [72], and also, unlike 3-dimensional bodies, due to their lower dimensionality, to their ability to relax by acquiring a variety of natural (stress-free) shapes, for instance, the wavy edges of growing leaves [42], the topological corrugations present on human brain [68], and the helical strands of DNA [18]. The present work is concerned with the central problem of formulating a general theory that takes under its ambit the non-Euclidean geometric characterization of these multifarious 2-dimensional defective structures and the subsequent determination of the stress fields and deformed shapes for a given distribution of material anomalies.

It is well established that differential geometry provides a rightful setting to describe the geometric nature of defects in 3-dimensional solids, as well as to discuss the related issues of strain incompatibility and residual stress distribution [1, 6, 13, 15, 34, 36, 39, 52, 69, 70]. Despite this success in 3 dimensions, the problem in lower dimensional structures is relatively less developed, primarily due to the complex interplay between the embedding geometries in the physical space, and the unavoidable non-linearities involved in the deformation as well as the constitutive responses. We note the initial attempts made by Eshelby [24, 25], who obtained analytical solutions for internal stress in linearly elastic plates containing isolated screw and edge dislocations, and subsequent generalizations by Chernykh [10] and Nabarro [48, 49], among others [47, 62, 64]. The notion of continuous distribution of defects in thin structures however has remained relatively unexplored outside the work of Povstenko [55, 56] and Zubov [73–75], where it was limited to only in-surface dislocations and disclinations (the difference between in-surface and out-of-surface defects is explained in Sect. 2). We also note that although the strain compatibility equations, both in the context of nonlinear Kirchhoff–Love shells [11, 12, 35, 53] and nonlinear Cosserat shells [20, 22, 44, 73], do exist, the strain incompatibility equations, with sources of incompatibility arising from a defect distribution, thermal deformation, or biological growth, etc., appear to be lacking in nonlinear shell theories. The incompatibility equations for Kirchhoff–Love plates, with only in-surface dislocations, has been derived, although with errors, by Derezin [16]. The incompatibility relations for a von-Kármán shallow shell theory have appeared in connection with thermal deformation [45], biological growth [17, 41–43], and surface defects in 2-dimensional crystals [8, 51]. The strain incompatibility equations have also appeared in the so called theories of non-Euclidean elastic plates [19, 30] which, without explicitly incorporating defect densities, consider a non-Euclidean metric, representing the distribution of a growth strain field, and use the Riemannian curvature of this metric as a measure of strain incompatibility to pose boundary-value-problems primarily for determining natural shapes.

Finally, we note some alternate attempts to investigate the mechanics of defective plates and shells [74, 75], of plastically deformed thin sheets [14, 67], and of biological growth in thin structures [46, 61], all of which do not use the notion of strain incompatibility.

We have extended the existing literature in several directions. First of all, we give a complete non-Euclidean characterization of all the translational, rotational, and metric anomalies in 2-dimensional structured continua. In doing so, we not only provide new insights into the geometrical nature of known defect densities, but also introduce various novel defect density measures in the context of structured surfaces (see Table 1 for a summary). Moreover, we use the well known Bianchi-Padova relations to discuss the interdependence of these densities as well as to obtain the relevant conservation laws. We also emphasize what distinguishes the nature of the surface defects from their 3-dimensional counterparts. Secondly, using concepts from non-Riemannian differential geometry, and incorporating the geometric character of defects, we derive the strain incompatibility relations for a nonlinear Cosserat shell with dislocations, disclinations, point defects, and other metric anomalies acting as sources of incompatibility. Finally, we reduce these general relations for Kirchhoff–Love shells and subsequently make certain smallness assumptions on strains and defect densities to obtain strain incompatibility conditions for sufficiently thin nonlinear shells with small surface strain but moderately large deformation. We use the simplified incompatibility relations within von-Kármán shell theory to discuss connections of our work with existing works on 2-dimensional crystalline surfaces, growth of biological membranes, and isotropic fluid films. This is to not only provide a rigorous basis to these existing theories but also to extend them to incorporate richer kinematics and defect structures. Our overall aim has been on one hand to unify several seemingly different streams of research, and on the other to provide a rigorously constructed and sufficiently general framework for studying a large range of problems associated with geometry and mechanics of defective structured surfaces.

A brief overview of the paper is as follows. In Sect. 2, we provide several illustrative examples to demonstrate the non-Euclidean character of local material defects in structured surfaces. In Sect. 3, we begin by introducing the notion of material space, which includes a 2-dimensional body manifold, a non-Riemannian material connection, and a material metric, as our prototype to characterize continuously defective structured surfaces. In particular, we use the tensors of non-metricity, torsion, and Riemann–Christoffel curvature of the material connection to construct several in-surface and out-of-surface material anomalies (see Table 1) and subsequently use Bianchi-Padova relations to emphasize their interdependence (see Table 2). We also introduce a Riemannian structure on the material space induced by the material metric and obtain geometric relations connecting the Riemannian and the non-Riemannian curvatures. In Sect. 4, a generalized notion of strain is introduced to establish the kinematical nature of our structured surface as a thin nonlinear Cosserat shell. The local strain compatibility equations are then discussed in detail, giving way to the local strain incompatibility relations with sources of incompatibility given in terms of various material anomalies. The central problem of stress and shape determination is taken-up next in Sect. 5 by restricting our attention to nonlinear Kirchhoff–Love shells with small surface strains but moderately large bending strains. In particular, we recover the Föppl–von-Kármán shell equations, with strain incompatibility as the source for stress and deformation, and illustrate how the incompatibility fields are related to defect densities and non-metricity. We provide several remarks drawing attention to the possible connection between our formalism and existing works before concluding our study in Sect. 6.

2 Geometric Nature of Surface Defects

Several illustrative examples of local defects in structured surfaces are now presented with an intent to emphasize the non-Euclidean geometric nature of the defects as is incorporated in the subsequent sections. In particular, the central idea of our work of embedding a 2-dimensional manifold, representing the defective structured surface, into a 3-dimensional non-Riemannian geometric space, with non-zero curvature, torsion, and non-metricity tensors,[1] emerges naturally as we proceed through these rudimentary illustrations. The nature of global anomalies are discussed in detail elsewhere [57, 58].

The *rotational anomalies* in a structured surface appear in the form of disclinations. Depending on the material nature of the surface, rotational order can be present due to intrinsic crystallinity of the surface (such as in colloidosomes, single-layer viral capsids, carbon nanotubes, and graphene) or due to an extrinsic orientation field (such as in nematic membranes, single layers in smectics, and cholesterics) [8, 33, 51]. As a result, we distinguish between rotational order, or lack thereof, appearing intrinsically and extrinsically in a surface. We also note that unlike disclinations in 3-dimensional crystalline solids, which have large formation energy and hence are rarely observed [5], disclinations in 2-dimensional crystals are omnipresent since the surface can now relax the energy by escaping into the third dimension. Isolated disclinations in structured surfaces with extrinsic rotational order are shown in Figs. 1(a, b). The rotational order is here present due to a director field distribution, denoted by $\boldsymbol{d}(\theta^1, \theta^2)$, over a planar domain parametrized by Cartesian coordinates (θ^1, θ^2). The director field in Fig. 1(a) is restricted to lie strictly in the $\theta^1\theta^2$-plane; it may represent deformed configuration of a nematic membrane or a single layer in the cholesteric phase of some liquid crystalline material [31, 32]. In contrast, the directors in Fig. 1(b) are allowed to orient themselves transversely to the plane; this can model either a lipid monolayer where the director orientation represents the orientation of individual lipid molecules, or a single layer of molecules in the smectic A or C phase [31, 32]. In lipid bilayers, nematics, and smectics, $\boldsymbol{d}$ is identifiable with $-\boldsymbol{d}$ due to the mirror symmetry about the mid-orthogonal plane of the director axis [31]. The lack of intrinsic crystalline order (translational and rotational), within the plane, in these examples can be primarily attributed to viscous relaxation [33]. Disclinations in such structured surfaces can be characterized by the signed angle through which the director rotates upon circumnavigating along a loop over the surface. The Frank vector $\boldsymbol{\omega}$ of the disclination is a precise measure of this signed angle. A disclination is of *wedge* or *twist* type depending on whether $\boldsymbol{\omega}$ is transverse or tangential, respectively, to the surface. The disclination in Fig. 1(a) is of wedge type with Frank vector $2\pi\mathbf{e}_3$ and the one in Fig. 1(b) is of twist type with Frank vector $2\pi\mathbf{e}_2$. Here, the triple $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ denote the standard basis of the Cartesian coordinate system $(\theta^1, \theta^2, \theta^3)$. Note that the wedge disclination line in Fig. 1(a) and the twist disclination line in Fig. 1(b) are both along the θ^3-axis. Disclinations can also appear in surfaces with intrinsic crystalline order, e.g., an ordered arrangement of lattice sites where the directors are attached in viral capsids or hexagonal lattice structure of the carbon atoms in graphene sheets [8, 51, 71]. As illustrated in Fig. 1(c), circumnavigating along a loop encircling the disclination, a lattice vector rotates through an angle which is an integral multiple of one of the rotational symmetry angles of the lattice. The wedge disclination located at O, in the 2-dimensional hexagonal lattice in Fig. 1(c), is characterized by its Frank vector $\boldsymbol{\omega} = (\pi/3)\mathbf{e}_3$. Material surfaces can also possess twist disclinations in the form of *local intrinsic orientational anomalies*, which correspond to breaking of the

[1] A Riemannian geometric space has zero torsion and non-metricity. A Euclidean geometric space has zero curvature, torsion, and non-metricity.

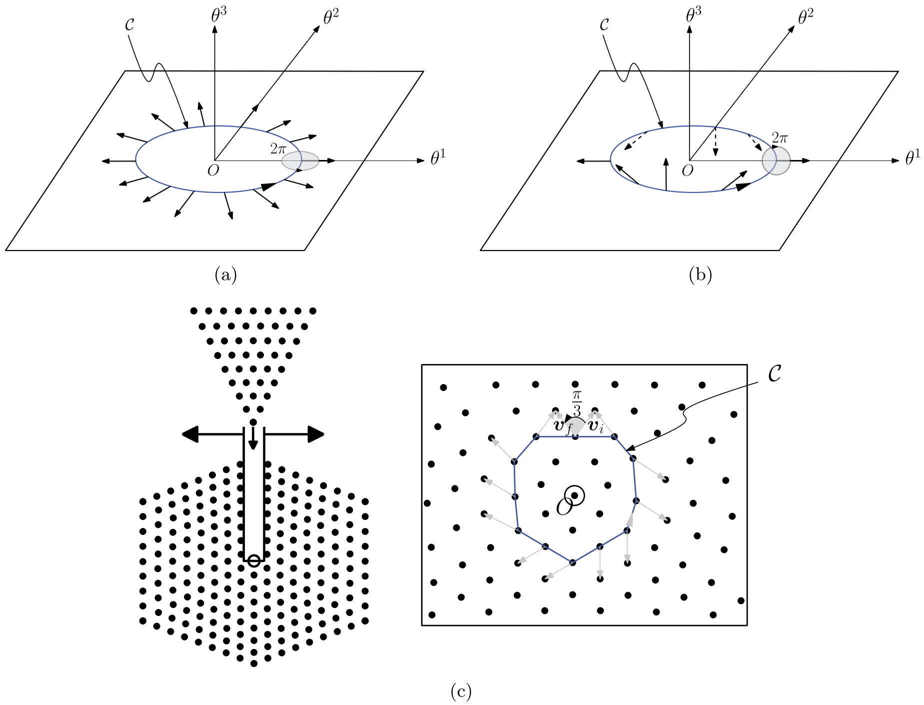


Fig. 1 (**a**) A single wedge disclination of Frank angle 2π in a nematic membrane, located at O, such that $\boldsymbol{d}(\theta^1, \theta^2) = \cos\theta \mathbf{e}_1 + \sin\theta \mathbf{e}_2$, where θ is the polar angle $\theta := \tan^{-1}(\theta^2/\theta^1)$; after [31]. (**b**) A single twist disclination of Frank angle 2π in a nematic shell, such that $\boldsymbol{d}(\theta^1, \theta^2) = \cos\theta \mathbf{e}_1 - \sin\theta \mathbf{e}_3$; after [31]. (**c**) Creation of a wedge disclination of Frank angle $\pi/3$ in a 2-dimensional hexagonal lattice by cutting the surface along a line and introducing a lattice wedge of angle $\pi/3$; after [5]. The marks on the surface represent lattice points which may carry identical atoms (in case of 2-dimensional crystals) or directors (in case of nematic shells) pointing inward/outward at the respective positions on the surface. The lattice vector, initially given by $\boldsymbol{v}_i$, rotates through an angle $\pi/3$ when circumnavigated along a loop surrounding the disclination

reflectional symmetries of the 2-dimensional material with the local tangent plane of the surface as the mirror plane, e.g., hemitropic plates [23, 66]. They are represented by an ill-defined (multi-valued) local orientation field over the surface. In order to quantify the disclinations discussed so far, the loop of circumnavigation is restricted within the surface. Indeed, the disclinations shown in Fig. 1, as well as the intrinsic orientational anomalies discussed above, are quantified using an in-surface loop $\mathcal{C}$. The case otherwise can appear in 2-dimensional homogenized models of thin 3-dimensional multi-layered structures, e.g., a stack of few monolayers of smectics or cholesterics, thin multi-walled nanotubes, or a thin slice of some 3-dimensional oriented media [32]. In these structures, disclinations may appear over the representative base surface (often the 'mid-surface' of the layered structure) as the homogenized or effective rotational anomaly of all the distributed disclinations across the thickness of the thin structure. In describing these disclinations, the loop of circumnavigation must be taken transversely to the base surface, see Fig. 2. Depending on the direction of the resulting vector of angular mismatch, these disclinations may either be of wedge or twist type. Finally, we note that disclinations often appear as dipoles, mainly due to energetic considerations; for instance, a single dipole of two oppositely signed wedge

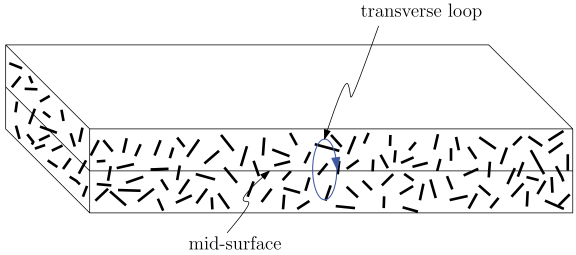


Fig. 2 A transverse loop characterizing an effectively 2-dimensional representation of the 3-dimensional distribution of disclinations within a thin layered structure made up of directed media

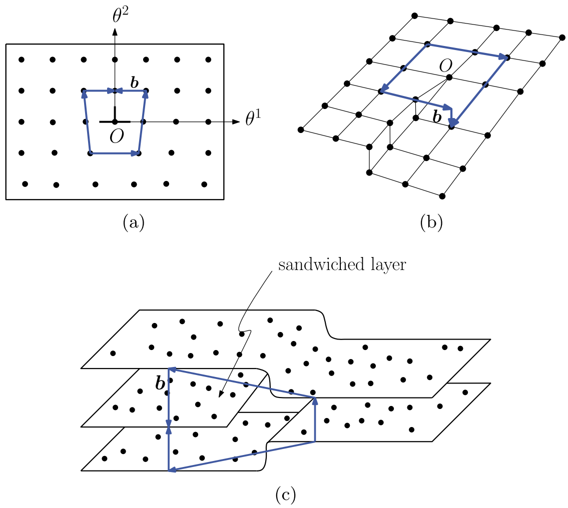


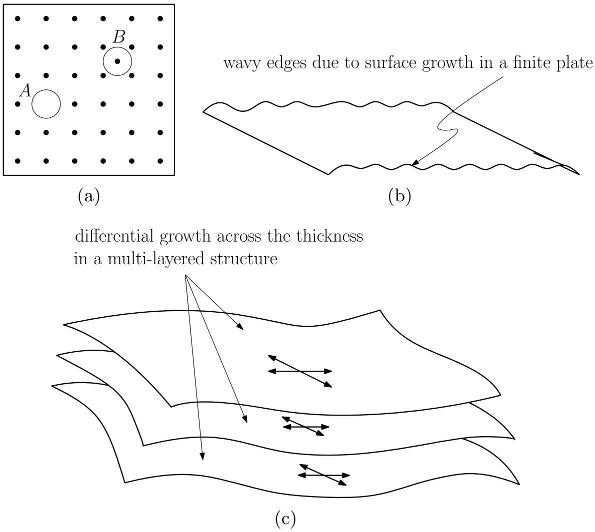
Fig. 3 (**a**) Isolated surface edge dislocation and (**b**) surface screw dislocation in a 2-dimensional cubic lattice. (**c**) Isolated edge dislocation in a thin multi-layered structure. The marks on the surface represent lattice points which may carry identical atoms as well as directors; after [33]

disclinations is geometrically and energetically equivalent to a single edge dislocation [5]. Such dipoles usually concentrate in arrays to form scars, grain boundaries, etc. [8].

The *translational anomalies* are represented by dislocations. The nature of dislocations in 2-dimensional matter is analogous to that in 3-dimensional materials. Isolated edge and screw dislocations are shown in Figs. 3(a) and 3(b), respectively, within a 2-dimensional cubic lattice along with the Burgers parallelograms. The Burgers vector, defined as the closure failure of the Burgers parallelogram, is tangential to the surface of the lattice in the former case and transverse in the latter. In these examples, the dislocations appear essentially due to the breaking of the intrinsic translational symmetries of the 2-dimensional matter [8, 51, 71]. On the other hand, in thin multi-layered structures or thin slices of oriented media, dislocations may be present, irrespective of the crystallinity of the material, as a result of either an order-mismatch of individual layers within the stack or as a homogenized or effective limit of all the distributed dislocations within the 3-dimensional slice [21]. The Burgers parallelogram is then transverse to the representative mid-surface of the stack, in contrast to the examples shown in Figs. 3(a, b). The precise type of these dislocations, edge or screw, can be determined from the direction of the Burgers vector. An edge dislocation in a layered medium is shown in Fig. 3(c), arising due to the presence of a sandwiched semi-infinite layer between two infinite layers of material [40, Ch. VI].

The *metrical anomalies* bring about ambiguity in the (local) notion of "length" and "angle" over the surface. Metric anomalies are generated due to intrinsic point imperfections such as vacancies and self-interstitials, see Fig. 4(a), as well as a result of in-surface thermal

Fig. 4 (**a**) A vacancy at position A and a self-interstitial at position B in a 2-dimensional cubic lattice. (**b**) Incompatible surface growth of a plate. (**c**) Differential growth of a thin multi-layered structure



deformation and biological growth [42, 43, 45, 51], see Fig. 4(b). Note that foreign interstitials fall within the realm of materially non-uniform bodies (e.g., functionally graded materials), not considered in the present work, where the material constitution changes from point to point. If the distance between the constituent entities in a lattice structure is measured by counting lattice steps, the presence of point defects, such as a vacancy or a self-interstitial, clearly introduces ambiguity in this step counting [39]. Apart from these pure in-surface metric anomalies, differential growth (or thermal deformation) across the thickness direction within a thin multi-layered structure may result in transverse metric anomalies within an appropriately homogenized 2-dimensional theory, see Fig. 4(c). These can be used to explain, for instance, the corrugations in human brain [68].

The simple examples described above are sufficient to motivate the non-Euclidean nature of the defects. Recall that, in order to quantify disclinations, we required circumnavigation of a vector along a loop and rotational mismatch between the initial and the final orientation of the vector. These notions correspond, respectively, to parallelly transporting a vector with respect to an affine connection and to the Riemann–Christoffel curvature associated with the affine connection [3]. The Frank vector $\boldsymbol{\omega}$ uniquely characterizes the Riemann–Christoffel curvature tensor. The related geometric space has to be necessarily non-Euclidean, since the director fields leading to disclinations are not parallel in the Euclidean sense. Moreover, as the directors may point outside the surface, a differential geometric description of disclinations in structured surfaces would necessarily require embedding the surface into a 3-dimensional Riemannian geometric space. In the case of dislocations, the closure failure of the Burgers parallelogram is analogous to the notion of torsion of an affine connection over a manifold which characterizes closure failures of infinitesimal parallelograms [6, 36]. Finally, the metric anomalies are characterized by the non-metricity tensor, which quantifies the non-uniformity of the metric tensor with respect to an appropriate affine connection [4, 37]. Incorporating dislocations and non-metricity would entail embedding the material surface in a non-Riemannian geometric space. Motivated by these geometric analogies, we are now in a position to pursue a systematic study of geometry of defects in a structured surface.

3 Geometric Characterization of Surface Defects

The mathematical prototype for structured surfaces is a connected, compact 2-dimensional manifold ω, possibly with boundary, which is embeddable (as a topological submanifold) in $\mathbb{R}^3$. Examples of such manifolds, in the orientable category, are sphere, sphere with a finite number of handles attached, twisted bands with $2n\pi$ twists for integers n etc.; and in non-orientable category, twisted bands with $(2n+1)\pi$ twists, e.g., a Möbius band for which n is zero. We can add boundaries to these manifolds by removing a finite number of open discs. The condition of embeddability in $\mathbb{R}^3$ precludes Klein bottle like surfaces and real projective planes. Our prototype manifold ω is topologically characterized by its orientability, twistedness, the number of open discs removed, i.e., the boundaries, and other topological invariants. We will call ω the *body manifold*. A fundamental theorem in differential topology (Tubular Neighbourhood Theorem [9, Theorem 11.4]) guarantees the existence of a *tubular neighbourhood* $\mathcal{M} := \{\boldsymbol{y} \in \mathbb{R}^3 \,|\, \mathrm{dist}(\omega, \boldsymbol{y}) < \epsilon, \epsilon > 0\}$ of ω in $\mathbb{R}^3$, for sufficiently small ϵ. Here, $\mathrm{dist}(\omega, \boldsymbol{y})$ denotes the minimum Euclidean distance of ω from $\boldsymbol{y}$. As a bounded open set in $\mathbb{R}^3$, $\mathcal{M}$ naturally admits a manifold structure, with ω as an embedded submanifold. Existence of $\mathcal{M}$ induces a vector bundle (the normal bundle) structure over ω [9], which entails a vector field $\boldsymbol{d} : \omega \to \mathbb{R}^3$ defined over ω. Our choice of ω, naturally endowed with a *director field* $\boldsymbol{d}$, is therefore appropriate for modelling structured surfaces. The differential structure, and all the fields to be defined over ω and $\mathcal{M}$, including $\boldsymbol{d}$, is assumed to be as smooth as the context demands.

Our strategy for characterizing material defects on a structured surface is to first equip $\mathcal{M}$ with a geometrical structure by associating with it a metric and an affine connection. This is then used to induce an appropriate non-Riemannian geometrical structure over ω, where various fundamental geometric objects, such as curvature, torsion, and non-metricity tensors, are interpreted as defect density measures. The induced metric and connection on ω is sufficient to encode all the information about the material structure of the structured surface [60]. While the geometric characterization of defects for 3-dimensional solids is well established [38, 39] (for a more recent review and a detailed bibliography see [60]), a similar attempt is missing for 2-dimensional material surfaces. In particular, we have collected here a wide variety of in-surface and out-of-surface anomalies, and have explained their non-Euclidean nature, only some of which appear otherwise in the existing literature on defective surfaces [8, 51, 55, 56]. Furthermore, the well known Bianchi-Padova relations are used to obtain several restrictions on the defect density fields. With these relations, it is emphasized that the various defect densities are in fact dependent on each other and follow certain conservation laws. The metric associated with $\mathcal{M}$ is also used to induce a Riemannian structure over ω. The relationship of the Riemann–Christoffel curvature tensor, associated with the affine connection, with the Riemann–Christoffel curvature tensor, obtained from the metric through the Levi-Civita connection, is derived. These relations subsequently provide the starting point for deducing the local strain incompatibility equations. They also lead to the well known local conditions under which ω is *locally isometrically* embeddable into $\mathbb{R}^3$, a notion that is related to the local compatibility of the strain fields.

In rest of the paper, lowercase Greek indices α, β, γ etc. take values from the set $\{1, 2\}$ and lowercase Roman indices i, j, k etc., from $\{1, 2, 3\}$. Einstein's summation convention holds over repeated indices unless specified otherwise. Round and square brackets enclosing indices indicate symmetrization and anti-symmetrization, respectively, with respect to them. The superscript (-1) is used to denote the inverse of an invertible matrix, whereas the superscript T is used to denote the transpose. The determinant and the trace of a matrix are denoted by det and tr, respectively.

3.1 Geometry on ω Induced from the Non-Riemannian Structure on $\mathcal{M}$: The Material Space

Let the 3-dimensional embedding manifold $\mathcal{M}$ be equipped with an affine connection $\mathfrak{L}$ and a metric $\boldsymbol{g}$. Consider a chart (V, θ^i) of $\mathcal{M}$ with $U := V \cap \omega \neq \emptyset$ such that the coordinates θ^α defined over $V \subset \mathcal{M}$ lie along U with $\zeta := \theta^3 \equiv 0$ at U. Such a coordinate system θ^i is called *adapted* to $U \subset \omega$. The restriction of the natural basis vector fields $\boldsymbol{G}_i$ over V to U will be denoted by $\boldsymbol{A}_i$, i.e., $\boldsymbol{A}_i(\theta^\alpha) := \boldsymbol{G}_i(\theta^\alpha, \zeta = 0)$, hence $\boldsymbol{A}_3$ is transverse to U. The coefficients of $\mathfrak{L}$ and the covariant components of $\boldsymbol{g}$ are denoted by L^i_{jk} and g_{ij}, respectively, with respect to $\boldsymbol{G}_i$. The covariant derivative of a sufficiently smooth vector field $\boldsymbol{u} = u^i(\theta^i)\boldsymbol{G}_i : V \to T_X V$, $X \in V$, with respect to $\mathfrak{L}$, is denoted by

$$u^i_{;j} := u^i_{,j} + L^i_{jk} u^k. \tag{1}$$

The notation ∇ is used for the surface covariant derivative of a tangent vector field $\boldsymbol{v} = v^\alpha(\theta^\alpha)\boldsymbol{A}_\alpha : U \to T_Y U$, $Y \in U$, with respect to the projection of $\mathfrak{L}$ on U, i.e., a connection with coefficients $L^\mu_{\alpha\nu}\big|_{\zeta=0}$,

$$\nabla_\alpha v^\mu := v^\mu_{,\alpha} + L^\mu_{\alpha\nu}\big|_{\zeta=0} v^\nu. \tag{2}$$

Here, the subscript $(\cdot)_{,i}$ denotes ordinary partial derivative with respect to θ^i. A vector field $\boldsymbol{u}$ along a curve over V is called *parallel* with respect to $\mathfrak{L}$ if, and only if, its covariant derivative along the curve vanishes identically.

The body manifold ω, equipped with connection $\mathfrak{L}$ and metric $\boldsymbol{g}$ from the embedding space $\mathcal{M}$, forms the *material space* $(\omega; \mathfrak{L}, \boldsymbol{g})$ of the structured surface. We will call $\mathfrak{L}$ the *material connection* and $\boldsymbol{g}$ the *material metric*. The "material" nature of these mathematical objects is due to the fact that the geometric quantities, given by curvature, torsion, and non-metricity tensors, derived from $\mathfrak{L}$ and $\boldsymbol{g}$, when restricted to $\zeta = 0$, represent various material anomalies within the material structure of the surface. Most importantly, we assume $\mathfrak{L}$ to be such that the curvature, torsion, and non-metricity tensors, defined over V, are uniform in the ζ coordinate and equal to their respective values at $\zeta = 0$, i.e., at $U \subset \omega$. This assumption alludes to the applicability of our model to thin multi-layered structures, or thin slices of defective media, represented as homogenized 2-dimensional surfaces. The 3-dimensional tubular neighborhood is therefore only a convenient extension of the defective material surface and should not be confused with a defective 3-dimensional body whose homogenization would otherwise lead to the considered material surface. It should also be noted that we are only looking at local defects and not the ones which could arise out of topological anomalies for multiply connected and non-orientable surfaces [57].

3.1.1 *Curvature of the Material Connection: Disclinations*

The components of the fourth-order Riemann–Christoffel curvature tensor of the material connection $\mathfrak{L}$ are given by [63, p. 138]

$$\tilde{\Omega}_{klj}{}^i := L^i_{lj,k} - L^i_{kj,l} + L^h_{lj} L^i_{kh} - L^h_{kj} L^i_{lh}. \tag{3}$$

The functions $\tilde{\Omega}_{klj}{}^i$ measure, in the linear approximation, the change that a vector, $\boldsymbol{v} \in T_X V$, $X \in V$, suffers under parallel transport with respect to $\mathfrak{L}$ along an infinitesimal loop $\mathcal{C}$ based at X and lying within V:

$$\delta v^i \approx -\frac{1}{2} \tilde{\Omega}_{klj}{}^i(X) v^j \oint_{\mathcal{C}} \theta^k d\theta^l, \tag{4}$$

where v^i are the components of the initial vector with respect to the basis $\boldsymbol{G}_i(X)$; the integral represents the infinitesimal area bounded by the loop $\mathcal{C}$. We define the purely covariant components $\tilde{\Omega}_{klji}$ by lowering the fourth index with the material metric g_{ij} as $\tilde{\Omega}_{klji} := g_{ip}\tilde{\Omega}_{klj}{}^p$. Clearly, $\tilde{\Omega}_{klj}{}^i = -\tilde{\Omega}_{lkj}{}^i$ and $\tilde{\Omega}_{klij} = -\tilde{\Omega}_{lkij}$. We assume $\tilde{\Omega}_{klij}(\theta^\alpha, \zeta) = \tilde{\Omega}_{klij}(\theta^\alpha, 0) =: \Omega_{klij}(\theta^\alpha)$, following the discussion in the previous paragraph.

It is useful to decompose the components $\Omega_{klij}(\theta^\alpha)$ into skew and symmetric parts [56]

$$\Omega_{klij} = \varepsilon_{pkl}\varepsilon_{qij}\Theta^{pq} + \varepsilon_{pkl}\zeta_{ij}{}^p, \tag{5}$$

where

$$\Theta^{pq} := \frac{1}{4}\varepsilon^{pij}\varepsilon^{qkl}\Omega_{ijkl} \quad \text{and} \quad \zeta_{ij}{}^p := \frac{1}{2}\varepsilon^{pkl}\Omega_{kl(ij)} \tag{6}$$

are components of the second-order tensor field $\boldsymbol{\Theta} = \Theta^{pq}\boldsymbol{A}_p \otimes \boldsymbol{A}_q$ and the third-order tensor field $\boldsymbol{\zeta} = \zeta_{ij}{}^k \boldsymbol{A}^i \otimes \boldsymbol{A}^j \otimes \boldsymbol{A}_k$. They represent, respectively, the skew part and the symmetric part of Ω_{klij} with respect to the last two indices. A geometric interpretation of these two fundamental tensors is as follows (see Fig. 5). Let the infinitesimal loop $\mathcal{C}$ in (4) be based at $X \in U \subset \omega$. Then, the change $\delta\boldsymbol{v}$ that a vector $\boldsymbol{v} \in T_X V$ undergoes when parallelly transported along $\mathcal{C}$, in the linear approximation, can be characterized by a second-order tensor $\boldsymbol{\beta} = \beta_{ij}\boldsymbol{A}^i \otimes \boldsymbol{A}^j$, i.e., $\delta\boldsymbol{v} = \boldsymbol{\beta}\boldsymbol{v}$, where

$$\beta_{ij} := -\frac{\delta A}{2}\Omega_{klij}\varepsilon^{rkl}n_r = -\delta A\,\varepsilon_{qij}\,\Theta^{pq}\,n_p - \delta A\,\zeta_{ij}{}^p\,n_p. \tag{7}$$

Here, δA is a measure of the infinitesimal area bounded by $\mathcal{C}$ and $\boldsymbol{n} = n_r\boldsymbol{A}^r$ its unit normal. The first term $W_{ij} := -\delta A\,\varepsilon_{qij}\,\Theta^{pq}\,n_p$ in the above expression is skew with axial vector $w^q = \Theta^{pq}\,n_p\,\delta A$. It represents the rotation that $\boldsymbol{v}$ has experienced under parallel transport about the axis $\boldsymbol{A}_p$, for each fixed p, probed by the three Euler angles Θ^{pq}. Thus, $\boldsymbol{\Theta}$ is the measure of the rotation of $\boldsymbol{v}$ about the axis $\boldsymbol{n}$. The second term $S_{ij} := -\delta A\,\zeta_{ij}{}^p\,n_p$, on the other hand, is symmetric; it represents a stretching, with the three principal values of the tensor $\boldsymbol{\zeta}\boldsymbol{n} = \zeta_{ij}{}^p n_p \boldsymbol{A}^i \otimes \boldsymbol{A}^j$ as measures of the stretch along their respective (linearly independent) principal directions. The tensor $\boldsymbol{\zeta}$ can be shown to be related to the metrical properties of $\mathcal{M}$ as it gives rise to a smeared out anomaly within the material structure which causes elongation or shortening of material vectors under parallel transport along loops, as shown in Fig. 5(a); it leads to what was termed as metrical disclination in our recent work [60]. We will assume $\boldsymbol{\zeta} \equiv \boldsymbol{0}$ in rest of the paper since, at present, we do not know of any defects in 2-dimensional materials which they would otherwise represent. The curvature tensor Ω_{klij} is then fully characterized in terms of the non-trivial independent components $\Omega_{[kl][ij]}$, i.e., the second-order tensor $\boldsymbol{\Theta}$. Some further consequences of neglecting metrical disclinations will be discussed in the next section.

We distinguish between two families of local rotational anomalies characterized by $\boldsymbol{\Theta}$. Consider, first, an infinitesimal loop $\mathcal{C}$ completely lying within U, see Fig. 5(b). Then, the i and j indices in Ω_{ijkl} can assume only values 1 and 2, and the resulting angular mismatch after parallel transport of arbitrary vectors is characterized by three fields

$$\Theta^q(\theta^\alpha) := \Theta^{3q}(\theta^\alpha) = \frac{1}{4}\varepsilon^{3\alpha\beta}\varepsilon^{qkl}\Omega_{\alpha\beta kl}. \tag{8}$$

These provide a measure for the distributed rotational anomalies within the material structure of the base manifold ω. Drawing analogy with Fig. 1, it is clear that the out-of-surface component Θ^3 provides a measure for the density of distributed wedge disclinations over the

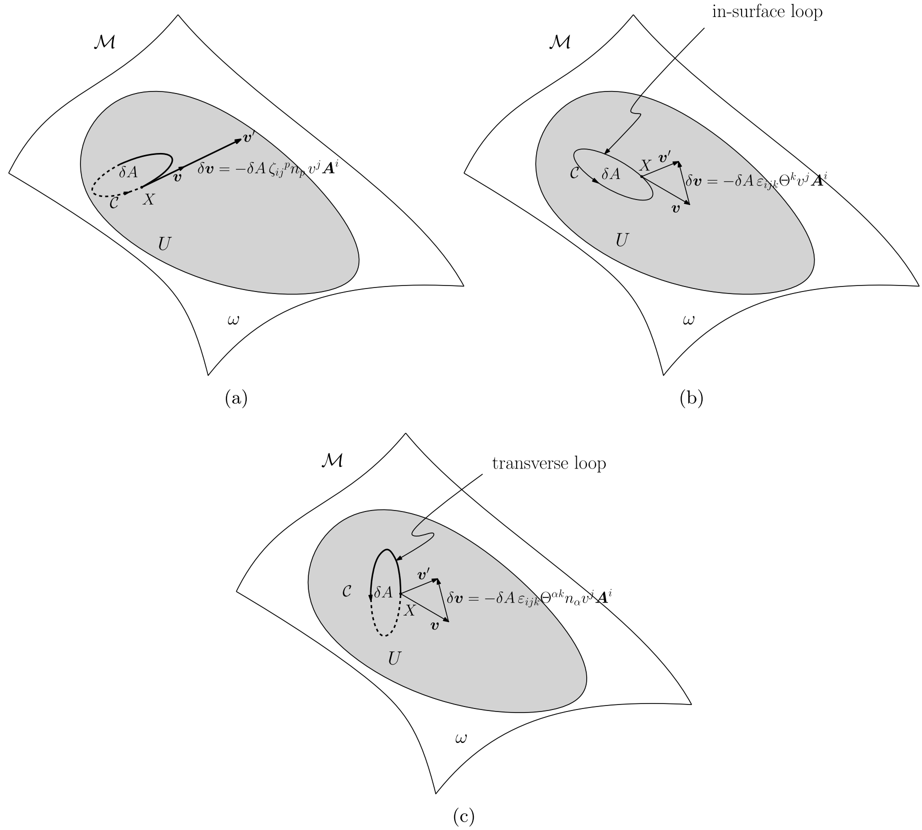


Fig. 5 (**a**) The symmetric part $\Omega_{ij(kl)}$, characterized by $\boldsymbol{\zeta}$, measures the stretching in $\boldsymbol{v} \in T_X V$, with $X \in U$, brought about by curvature of the material space. Here, $\boldsymbol{v}$ is a principal direction of the second-order tensor $\boldsymbol{\zeta n}$ and $\boldsymbol{n}$ is the unit normal to the infinitesimal area element δA bounded by the loop $\mathcal{C}$. The purely rotational change in $\boldsymbol{v} = v^i \boldsymbol{A}_i$, brought about by the curvature tensor, is measured by (**b**) the skew part $\Omega_{\alpha\beta[ij]}$, characterized by $\Theta^i \boldsymbol{A}_i$, when $\mathcal{C}$ is completely within U, and (**c**) the skew part $\Omega_{\alpha 3[ij]}$, characterized by $\Theta^{\alpha q} \boldsymbol{A}_\alpha \otimes \boldsymbol{A}_q$, whenever $\mathcal{C}$ is transverse to U

structured surface [8, 51, 55], see Figs. 1(a, c), irrespective of its crystallinity, whereas the in-surface components Θ^μ characterize either the distributed intrinsic orientational anomalies, in case of intrinsically crystalline surfaces, or distributed twist disclinations, in case of directed surfaces (as shown in Fig. 1(b)). Next, we consider $\mathcal{C}$, based at $X \in U$, to lie transversely to U, see Fig. 5(c). One of the indices i and j in Ω_{ijkl} will then take the value 3, and the resulting angular mismatch after parallel transport of arbitrary vectors is characterized by the remaining six independent components of $\boldsymbol{\Theta}$:

$$\Theta^{\alpha q} = \frac{1}{4} \varepsilon^{\alpha\mu 3} \varepsilon^{qkl} \Omega_{\mu 3kl}. \tag{9}$$

Recalling our discussion in Sect. 2 on disclinations in thin multi-layered structures of oriented media, see also Fig. 2, we conclude that these components provide a measure for a variety of homogenized/effective rotational anomalies of the distributed disclinations across the thickness of the multi-layered structured surface. Out of these six functions, Θ^{11} and

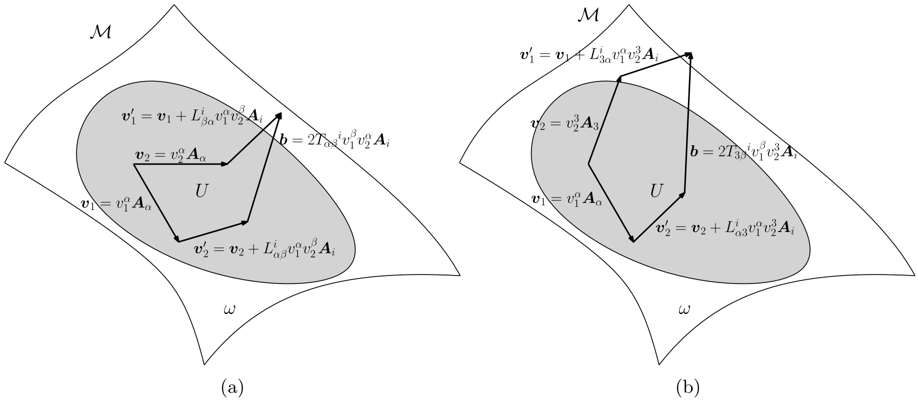


Fig. 6 (**a**) Closure failure of an infinitesimal in-surface parallelogram due to the $T_{\alpha\beta}{}^i$ components of the torsion tensor. (**b**) Closure failure of an infinitesimal transverse parallelogram due to the $T_{\alpha 3}{}^i$ components of the torsion tensor

Θ^{22} are of wedge type, and Θ^{12}, Θ^{21}, and $\Theta^{\alpha 3}$ are of twist type. As we will see shortly, in Sect. 3.1.4, these densities are in fact dependent on each other.

3.1.2 Torsion of the Material Connection: Dislocations

Consider two tangent vectors $\boldsymbol{v}_1 = v_1^i \boldsymbol{A}_i$, $\boldsymbol{v}_2 = v_2^i \boldsymbol{A}_i$ at some point Y on U. Translating $\boldsymbol{v}_1$ parallelly along $\boldsymbol{v}_2$ and $\boldsymbol{v}_2$ along $\boldsymbol{v}_1$ with respect to $\mathfrak{L}$, we obtain the vectors

$$\boldsymbol{v}_1' = \boldsymbol{v}_1 + L^i_{jk}\big|_{\zeta=0} v_1^k v_2^j \boldsymbol{A}_i \quad \text{and} \quad \boldsymbol{v}_2' = \boldsymbol{v}_2 + L^i_{kj}\big|_{\zeta=0} v_1^k v_2^j \boldsymbol{A}_i, \tag{10}$$

respectively. The closure failure of the parallelogram is given by (see Fig. 6)

$$\boldsymbol{b} = \boldsymbol{v}_2 + \boldsymbol{v}_1' - \boldsymbol{v}_1 - \boldsymbol{v}_2' = 2T_{jk}{}^i\left(\theta^\alpha\right) v_1^k v_2^j \, \boldsymbol{A}_i, \tag{11}$$

where the functions

$$T_{jk}{}^i\left(\theta^\alpha\right) := L^i_{[jk]}|_{\zeta=0} \tag{12}$$

constitute the components of the third-order torsion tensor (anti-symmetric in the lower indices) over U [63, p. 126]. We assume that $\tilde{T}_{jk}{}^i(\theta^\alpha, \zeta) = \tilde{T}_{jk}{}^i(\theta^\alpha, 0)$, where $\tilde{T}_{jk}{}^i := L^i_{[jk]}$, which in turn is same as $T_{jk}{}^i(\theta^\alpha)$. Associated with the torsion tensor, we have the second-order axial tensor

$$\alpha^{ij}\left(\theta^\alpha\right) := \frac{1}{2}\varepsilon^{ikl}\left(\theta^\alpha\right) T_{kl}{}^j\left(\theta^\alpha\right). \tag{13}$$

Here, $\varepsilon^{ijk}(\theta^\alpha) := g^{-\frac{1}{2}} e^{ijk}$, where $e^{ijk} = e_{ijk}$ is the 3-dimensional permutation symbol and $g := \det[g_{ij}\big|_{\zeta=0}]$. For later use, we define $\varepsilon_{ijk}(\theta^\alpha) := g^{\frac{1}{2}} e_{ijk}$. The components α^{ij} provide measures for a variety of dislocation distributions over the structured surface. Taking $v_1^3 = v_2^3 = 0$ (i.e., $\boldsymbol{v}_1$ and $\boldsymbol{v}_2$ tangential to U, see Fig. 6(a)), and comparing with Figs. 3(a, b), it is immediate that

$$J^\alpha := \alpha^{3\alpha} = \frac{1}{2}\varepsilon^{\mu\nu 3} T_{\mu\nu}{}^\alpha \tag{14}$$

represent a distribution of in-surface edge dislocations and

$$J^3 := \alpha^{33} = \frac{1}{2}\varepsilon^{\mu\nu 3} T_{\mu\nu}{}^3 \tag{15}$$

a distribution of in-surface screw dislocations [55, 56]. Next, taking $v_1^3 = v_2^\alpha = 0$ (i.e., $\boldsymbol{v}_1$ tangential and $\boldsymbol{v}_2$ transverse to U, see Fig. 6(b)), and comparing with Fig. 3(c), it is evident that the components $\alpha^{\mu k} := \frac{1}{2}\varepsilon^{3\alpha\mu} T_{3\alpha}{}^k$, with α^{11}, α^{22} as the screw components and α^{12}, $\alpha^{\mu 3}$ as the edge components, represent the out-of-surface dislocations in thin multi-layered oriented media such as those discussed in Sect. 2.

3.1.3 Non-metricity of the Material Connection: Metric Anomalies

The third-order non-metricity tensor of the material space, measuring non-uniformity of the metric $\boldsymbol{g}$ with respect to the connection $\mathfrak{L}$, has covariant components $\tilde{Q}_{kij}$ defined as [63, p. 131]

$$\tilde{Q}_{kij} := -g_{ij;k} = -g_{ij,k} + L^p_{ki} g_{pj} + L^p_{kj} g_{ip}. \tag{16}$$

The negative sign in the definition is conventional. The second equality in (16) follows from the definition of the covariant derivative. We assume that $\tilde{Q}_{kij}(\theta^\alpha, \zeta) = \tilde{Q}_{kij}(\theta^\alpha, 0) =: Q_{kij}(\theta^\alpha)$. The pure in-surface components $Q_{\alpha\mu\nu}$ provide measure for the distributed surface metric anomalies, whereas components Q_{kij}, with either of k, i or j taking the value 3, indicate the presence of out-of-surface metric anomalies, e.g., thickness-wise growth. A non-zero $Q_{\alpha\mu\nu}$ leads to variation in the angle between tangent vectors during parallel transport with respect to the projected connection $L^\alpha_{\beta\gamma}\big|_{\zeta=0}$, see Fig. 7(a). Indeed, the inner product $\boldsymbol{g}\big|_{\zeta=0}(\boldsymbol{u}, \boldsymbol{w}) = a_{\alpha\beta} u^\alpha v^\beta$ of two tangent vectors $\boldsymbol{u} = u^\alpha \boldsymbol{A}_\alpha$ and $\boldsymbol{v} = v^\alpha \boldsymbol{A}_\alpha$, where $a_{\alpha\beta}(\theta^\alpha) := g_{\alpha\beta}(\theta^\alpha, \zeta = 0)$, changes under parallel transport with respect to $L^\alpha_{\beta\gamma}\big|_{\zeta=0}$ from the initial point $C^\alpha(0)$ to any generic point $C^\alpha(s)$, along some parametrized curve $\mathcal{C} = C^\mu(s) \boldsymbol{A}_\mu(\theta^\alpha(s))$ lying over U, by the amount

$$\begin{aligned} a_{\alpha\beta} u^\alpha v^\beta(s) - a_{\alpha\beta} u^\alpha v^\beta(0) &= \int_0^s \left(a_{\alpha\beta} u^\alpha v^\beta\right)_{,\mu}(\tau)\, \dot{C}^\mu(\tau)\, d\tau \\ &= -\int_0^s Q_{\mu\alpha\beta}\big(\theta^\alpha(\tau)\big) u^\alpha(\tau) v^\beta(\tau)\, \dot{C}^\mu(\tau)\, d\tau. \end{aligned} \tag{17}$$

Here, we have used, $u^\alpha_{;\mu}\big|_{\zeta=0} \dot{C}^\mu \equiv 0$ and $v^\beta_{;\mu}\big|_{\zeta=0} \dot{C}^\mu \equiv 0$ throughout $\mathcal{C}$, as they are parallelly transported fields along $\mathcal{C}$, where $\dot{C}^\mu(s)$ denotes the ordinary derivative of $C^\mu(s)$ with respect to its argument. In structured surfaces, as we have earlier discussed in Sect. 2, this variation in inner product, characterized above in terms of a non-trivial $Q_{\alpha\mu\nu}$, may arise from a distribution of point imperfections in the arrangement of molecules or atoms over the surface, e.g., vacancies and self-interstitials in 2-dimensional crystals, inserting (or removing) a lipid molecule into (or out of) a crystalline arrangement of identical molecules over a monolayer, thermal deformation of the surface, biological growth of cell membranes, leaves etc. The remaining components $Q_{3ij} = -g_{ij;3}\big|_{\zeta=0}$ and $Q_{\mu i3} = -g_{i3;\mu}\big|_{\zeta=0}$ measure the non-uniformity of the material metric in the ζ-direction, i.e., along the thickness of the structured surface, and the change in length of transverse vectors along the surface, respectively, see Figs. 7(b) and 7(c). These provide faithful representations for differential growth along the thickness in thin multi-layered structures discussed in Sect. 2 and illustrated in Fig. 4(c).

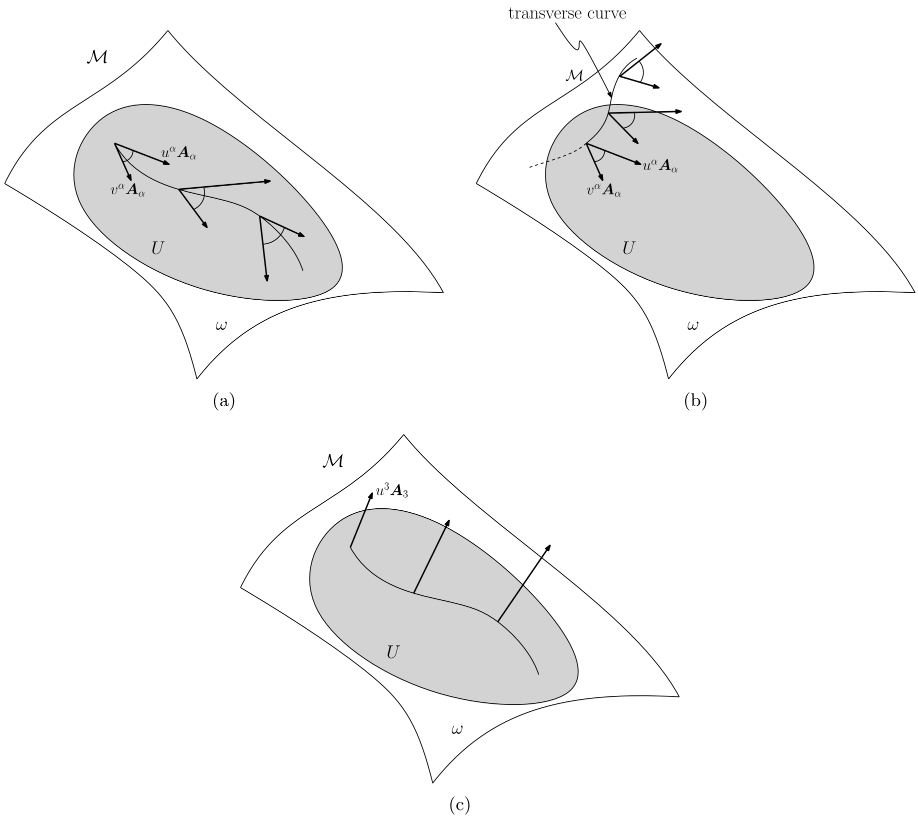


Fig. 7 (**a**) Change in angle between two vectors, tangent to U, due to non-zero $Q_{\mu\alpha\beta}$. (**b**) Change in angle between two vectors along a transverse curve due to non-zero Q_{3ij}. (**c**) Change in length of a transverse vector along a surface curve due to non-zero $Q_{\mu i3}$

The set of all defect densities are summarized in Table 1. The densities Θ^3, Θ^μ, J^μ, J^3 have appeared previously in [55] whereas a very special semi-metric form of $\zeta_{ij}{}^k$ and $Q_{\mu\alpha\beta}$ has appeared in [56], however without much insight into their geometrical nature, cf. [7, 16, 74, 75]. On the other hand, Θ^3, J^μ, and an isotropic form of $Q_{\mu\alpha\beta}$ (see below) has been considered in the condensed matter literature [8, 51], although only in the sense of smeared-out distributions of discrete defects. The out-of-surface densities $\Theta^{\mu k}$ and $\alpha^{\mu k}$, metrical disclinations $\zeta_{ij}{}^k$, and anisotropic non-metricity, have not appeared elsewhere in the context of defective surfaces.

3.1.4 Bianchi-Padova Relations

The tensors of curvature, torsion, and non-metricity of a non-Riemannian space cannot be arbitrary due to geometric restrictions. Besides the restrictions $\tilde{Q}_{k[ij]} = 0$, $\tilde{T}_{(ij)}{}^k = 0$, and $\tilde{\Omega}_{(ij)kl} = 0$, which follow from the definitions of these quantities, the following system of differential relations, known as the Bianchi-Padova relations [63, p. 144], are identically satisfied:

$$2\tilde{T}_{[jk}{}^{l}{}_{;i]} = \tilde{\Omega}_{[ijk]}{}^{l} + 4\tilde{T}_{[ij}{}^{p}\,\tilde{T}_{k]p}{}^{l}, \tag{18a}$$

Table 1 Non-Riemannian geometric objects on ω and the defects they characterize in structured surfaces

Geometric objects	Defect densities
$\Theta^3 := \Theta^{33}$	In-surface wedge disclinations; Figs. 1(a, c) and 5(b)
$\Theta^\mu := \Theta^{3\mu}$	In-surface twist disclinations or intrinsic orientational anomalies; Figs. 1(b) and 5(b)
$\Theta^{\mu k}$	Disclinations associated with transverse loops; Figs. 2 and 5(c)
$\zeta_{ij}{}^k$	Metrical disclinations; Fig. 5(a)
$J^\mu := \alpha^{3\mu}$	In-surface edge dislocations; Figs. 3(a) and 6(a)
$J^3 := \alpha^{33}$	In-surface screw dislocations; Figs. 3(b) and 6(a)
$\alpha^{\mu k}$	Out-of-surface dislocations; Figs. 3(c) and 6(b)
$Q_{\mu\alpha\beta}$	In-surface metric anomalies; Figs. 4(a, b) and 7(a)
Q_{3ij} and $Q_{\alpha i3}$	Out-of-surface metric anomalies; Figs. 4(c) and 7(b, c)

$$\tilde{\Omega}_{[jk|l|}{}^p{}_{;i]} = 2\tilde{T}_{[ij}{}^q\,\tilde{\Omega}_{k]ql}{}^p, \quad \text{and} \tag{18b}$$

$$\tilde{Q}_{[j|kl|;i]} = \tilde{T}_{ij}{}^p\,\tilde{Q}_{pkl} - \tilde{\Omega}_{ij(kl)}. \tag{18c}$$

In the above expressions, anti-symmetrization with respect to three indices is defined as

$$A_{[nml]\cdots}{}^{\cdots} := \frac{1}{6}\big(A_{nml\cdots}{}^{\cdots} + A_{lnm\cdots}{}^{\cdots} + A_{mln\cdots}{}^{\cdots} - A_{lmn\cdots}{}^{\cdots} - A_{nlm\cdots}{}^{\cdots} - A_{mnl\cdots}{}^{\cdots}\big). \tag{19}$$

The enclosed indices within two vertical bars in the subscript are to be exempted from anti-symmetrization. Clearly, $A_{[\alpha\beta\mu]\cdots}{}^{\cdots} = 0$ and $A_{[nnl]\cdots}{}^{\cdots} = 0$ (no summation on n). Additionally, there is a fourth Bianchi-Padova relation [63, p. 145], purely algebraic in nature, based on the following identity satisfied by the components of any fourth-order tensor $\tilde{\Omega}_{ijkl}$ with $\tilde{\Omega}_{(ij)kl} = 0$:

$$\tilde{\Omega}_{ijkl} - \tilde{\Omega}_{klij} = -\frac{3}{2}\big(\tilde{\Omega}_{[jik]l} + \tilde{\Omega}_{[jlk]i} + \tilde{\Omega}_{[lik]j} + \tilde{\Omega}_{[ijl]k}\big) + \tilde{\Omega}_{kj(li)} + \tilde{\Omega}_{ik(lj)} + \tilde{\Omega}_{jl(ik)} + \tilde{\Omega}_{li(jk)} + \tilde{\Omega}_{lk(ji)} + \tilde{\Omega}_{ij(lk)}. \tag{20}$$

After substituting relations (18a) and (18c) into (20), it boils down to an expression for $\tilde{\Omega}_{ijkl} - \tilde{\Omega}_{klij}$ in terms of $\tilde{T}_{ij}{}^k$, $\tilde{Q}_{kij}$, $\tilde{T}_{[jk}{}^l{}_{;i]}$, and $\tilde{Q}_{[j|kl|;i]}$. For a torsion-free, metric-compatible ($\tilde{Q}_{kij} = 0$) connection (i.e., a Levi-Civita connection), this implies the familiar symmetry $\tilde{\Omega}_{ijkl} = \tilde{\Omega}_{klij}$. However, as shown below, this particular symmetry can be achieved in sufficiently thin structures under less restrictive conditions. The linearized form of the first three Bianchi-Padova relations, restricted to the surface and considering only the in-surface anomalies, has been mentioned by Povstenko [55, 56], but without noting their implications, some of which are studied below.

Consequences of the first Bianchi-Padova relation: Equation (18a) is non-trivial only when at least one of the indices i, j and k assume the value 3, since otherwise $A_{[\alpha\beta\mu]} = 0$. Recalling our assumption that $\tilde{T}_{ij}{}^k$ is uniform with respect to the ζ coordinate, (18a) reduces to

$$4\nabla_{[\beta}T_{|3|\alpha]}{}^l = -\big(\Omega_{\alpha\beta3}{}^l + \Omega_{3\alpha\beta}{}^l - \Omega_{3\beta\alpha}{}^l\big) - 4\big(T_{\alpha\beta}{}^\mu T_{3\mu}{}^l + T_{3\alpha}{}^p T_{\beta p}{}^l - T_{3\beta}{}^p T_{\alpha p}{}^l\big). \tag{21}$$

Furthermore, if we assume that the structured surface is sufficiently thin such that there are no dislocations associated with the transverse Burgers parallelograms, i.e., $\alpha^{\mu k}=0$ (the in-surface dislocations J^i can still be present), then (21) simplifies into a system of algebraic equations:

$$\Omega_{\alpha\beta 3l}=\Omega_{3\beta\alpha l}-\Omega_{3\alpha\beta l}. \tag{22}$$

For $l=3$, we obtain $\Omega_{3\beta\alpha 3}=\Omega_{3\alpha\beta 3}$, since $\Omega_{\alpha\beta 33}=0$ (from $\boldsymbol{\zeta}=\mathbf{0}$). This is equivalent to $\Omega_{\beta 3\alpha 3}=\Omega_{\alpha 3\beta 3}$, or

$$\Theta^{\alpha\beta}=\Theta^{\beta\alpha}. \tag{23}$$

For $l=\mu$, (22) can be rewritten as $\Omega_{\alpha\beta 3\mu}=\Omega_{3\beta\alpha\mu}-\Omega_{3\alpha\beta\mu}$, or equivalently

$$\Theta^{3\mu}=\Theta^{\mu 3}. \tag{24}$$

Combining the above two relations we can therefore infer that, for vanishing $\alpha^{\mu k}$, the disclination density tensor $\boldsymbol{\Theta}$ is symmetric. Moreover, due to (8), $\Theta^{\mu}=\Theta^{\mu 3}$, i.e., the pure in-surface disclination densities Θ^{μ} (which may either characterize densities of twist disclinations in directed surfaces or intrinsic orientational anomalies in hemitropic surfaces) should be identical to the wedge disclination densities $\Theta^{\mu 3}$ associated with transverse loops, e.g., in multi-layered surfaces as discussed in Sect. 2; in particular, they should vanish in sufficiently thin structured surfaces, e.g., in 2-dimensional crystals, where both $\Theta^{\mu 3}$ and $\alpha^{\mu k}$ will be absent. We note that, in contrast, for 3-dimensional solids, the symmetry of the disclination density tensor is implied only under vanishing of the full torsion and the non-metricity tensor. It is worthwhile to reemphasize that the assumption $\alpha^{\mu k}=0$ is realistic only in sufficiently thin structures such as biological membranes and graphene sheets, among others. On the other hand, if we consider multi-layered or moderately thin structures of oriented media, where the assumption of vanishing $\alpha^{\mu k}$ is no longer physical, and assume that they do not contain any disclinations and metric anomalies, and also that J^i and $\alpha^{\mu k}$ are small (of the same order), then (21) yields

$$\nabla_{\mu}\alpha^{\mu k}=0. \tag{25}$$

This is a conservation law for the $\alpha^{\mu k}$-type dislocations enforcing that they must always form loops or leave the surface. In either case, whether the $\alpha^{\mu k}$-dislocations are absent or not, there is no restriction on the in-surface dislocation densities J^i. This again is in contrast to 3-dimensional solids, where the first Bianchi-Padova relation provides a conservation law for all dislocation densities [56, 60].

Consequences of the second Bianchi-Padova relation: Equation (18b), in the absence of both $\alpha^{\mu q}$-type dislocations and metric anomalies ($Q_{ijk}=0$), in addition to $\boldsymbol{\zeta}=\mathbf{0}$, reduces to a simple conservation law

$$\nabla_{\mu}\Theta^{\mu k}=2\varepsilon_{3\mu\nu}J^{\mu}\Theta^{\nu k}, \tag{26}$$

to be satisfied by disclinations characterized by $\Theta^{\mu k}$, as well as $\Theta^{k\mu}$ owing to the symmetries $\Theta^{\mu k}=\Theta^{k\mu}$ (see (23) and (24)), and surface edge dislocations. Assuming that J^{α} and $\Theta^{\mu k}=\Theta^{k\mu}$ are small, and of the same order, we obtain

$$\nabla_{\mu}\Theta^{\mu k}=\nabla_{\mu}\Theta^{k\mu}=0. \tag{27}$$

These are linear conservation laws for the respective disclinations, requiring their lines to either form loops or leave the surface. Note that there is no restriction on Θ^3 (wedge disclinations), in contrast to what one would expect for 3-dimensional solids.

Consequences of the third Bianchi-Padova relation: We use (18c) to obtain a simple representation for the non-metricity tensor. With $\boldsymbol{\zeta} = \mathbf{0}$, (18c) can be rewritten as

$$\left(\tilde{Q}_{jkl,i} + L^p_{jk}\tilde{Q}_{ipl} + L^p_{jl}\tilde{Q}_{ipk}\right)_{[ji]} = 0. \tag{28}$$

It can be shown by direct substitution that a non-trivial solution of (28) is given by

$$\tilde{Q}_{kij} = -2\tilde{q}_{ij;k}, \tag{29}$$

where $\tilde{q}_{ij} = \tilde{q}_{ji}$ are arbitrary symmetric functions over V. It is a consequence of the fundamental existence theorem of linear differential systems that, in absence of disclinations (i.e., $\Omega_{ijkl} = 0$) over a simply connected U (hence V), if the matrix field $\bar{g}_{ij} := g_{ij} - 2\tilde{q}_{ij}$ is positive-definite for symmetric functions $\tilde{q}_{ij} = \tilde{q}_{ji}$, then $\tilde{Q}_{kij} = -2q_{ij;k}$ is the only solution to (28) over V [60]. As the density of metric anomalies is assumed to be uniform with respect to the ζ coordinate, we will interpret this representation of the metric anomalies in absence of disclinations over simply connected patches over ω as

$$Q_{kij}(\theta^\alpha) = -2\tilde{q}_{ij;k}\big|_{\zeta=0}. \tag{30}$$

The symmetric matrix field $\tilde{q}_{ij}$ is known as quasi-plastic strain [4]. In the absence of disclinations, the positive-definite symmetric matrix field $\bar{g}_{ij}$ can be used to define an *auxiliary material space* $(\omega, \mathfrak{L}, \bar{\boldsymbol{g}})$, equipped with the original material connection $\mathfrak{L}$ but a metric $\bar{\boldsymbol{g}}$. The non-metricity of the auxiliary material space vanishes identically by definition. The second-order tensor field $\boldsymbol{q} := q_{\mu\nu}\boldsymbol{A}^\mu \otimes \boldsymbol{A}^\nu$, where $q_{\mu\nu}(\theta^\alpha) := \tilde{q}_{\mu\nu}(\theta^\alpha, \zeta = 0)$, characterizing the pure in-surface metric anomalies in the absence of disclinations, can be uniquely decomposed as

$$q_{\mu\nu} = \lambda a_{\mu\nu} + \mathfrak{q}_{\mu\nu}, \tag{31}$$

where $\lambda := \frac{1}{2}q^\mu{}_\mu = \frac{1}{2}a^{\mu\alpha}q_{\alpha\mu}$ is the dilatational part of $q_{\mu\nu}$ and $\mathfrak{q}_{\mu\nu}$ is the deviatoric part of $q_{\mu\nu}$ (i.e., $\mathfrak{q}^\mu{}_\mu = 0$). The first term represents isotropic metric anomalies and the second represents anisotropic metric anomalies [60]. This general form of non-metricity is readily applicable to model various real-life surface metric anomalies such as 2-dimensional anisotropic biological growth, thermal expansion, distributed point defects, etc. When $\boldsymbol{q}$ is purely isotropic, i.e., $q_{\mu\nu} = \lambda a_{\mu\nu}$, it is straightforward to obtain $Q_{\alpha\mu\nu} = -\mu_{,\alpha}a_{\mu\nu}$, where $\mu := \ln(1 + 2\lambda)$. The surface metric of the auxiliary material space for isotropic metric anomalies is, hence, conformal to the surface metric of the original material space, $\bar{a}_{\mu\nu} = (1 + 2\lambda)a_{\mu\nu}$.

Consequences of the fourth Bianchi-Padova relation: The fourth Bianchi-Padova relation imposes interdependence on the disclination density measures Θ^{pq}. Assuming $\boldsymbol{\zeta} = \mathbf{0}$, the in-surface components of (20) require $\Omega_{\alpha\beta\mu\nu} - \Omega_{\mu\nu\alpha\beta} = 0$, since $A_{[\alpha\beta\mu]\dots} = 0$, which is the trivial relation $\Theta^{33} = \Theta^{33}$. Next, if we also assume that the metric anomalies are absent, i.e., $Q_{kij} = 0$, then (20), together with (18a), yields

$$\begin{aligned}\Omega_{\alpha j\mu 3} - \Omega_{\mu 3\alpha j} = -3\big(&T_{[3\mu|\alpha|;j]} - 2T_{[j3}{}^iT_{\mu]i\alpha} + T_{[\alpha\mu|j|;3]} - 2T_{[3\alpha}{}^iT_{\mu]ij}\\ &+ T_{[j3|\mu|;\alpha]} - 2T_{[\alpha j}{}^iT_{3]i\mu}\big),\end{aligned} \tag{32}$$

where, $T_{ijp} := T_{ij}{}^kg_{kp}$. After substituting $T_{ijk;3} = 0$, as per our restriction on $\mathfrak{L}$, and assuming in addition $T_{3\alpha}{}^i = 0$, or equivalently $\alpha^{\mu k} = 0$, the right-hand-side of the above relation vanishes identically, thereby enforcing the symmetries

$$\Omega_{\alpha\beta\mu 3} - \Omega_{\mu 3\alpha\beta} = 0 \quad \text{and} \quad \Omega_{\alpha 3\mu 3} - \Omega_{\mu 3\alpha 3} = 0. \tag{33}$$

Table 2 Symmetries, conservation laws, and representations of defect density fields imposed by the Bianchi-Padova relations

Symmetries and conservation laws from Bianchi-Padova relations with ${\zeta_{ij}}^k \equiv 0$	Implications on defect densities
$\alpha^{\mu k} = 0 \Rightarrow \Theta^{ij} = \Theta^{ji}$	The two distinct families of disclinations Θ^{3i} and $\Theta^{\alpha i}$ are dependent on each other
$\{\Theta^{ij} = 0$, $Q_{kij} = 0$, and $\alpha^{\mu k}$, J^i small$\} \Rightarrow \nabla_\mu \alpha^{\mu k} = 0$	$\alpha^{\mu k}$-dislocations either form loops or leave the surface
$\{\alpha^{\mu k} = 0$, $Q_{kij} = 0$, J^α and $\Theta^{\mu k} = \Theta^{k\mu}$ small$\} \Rightarrow \nabla_\mu \Theta^{\mu k} = \nabla_\mu \Theta^{k\mu} = 0$	Disclinations associated with the transverse loops, either form loops or leave the surface
On simply connected domains on ω, with $\Theta^{ij} = 0$, $Q_{kij} = -2\tilde{q}_{ij;k}\big\vert_{\zeta=0}$	Non-metricity Q_{kij} can be represented in terms of a symmetric second-order tensor

In terms of disclination densities, these are, respectively, $\Theta^{3\mu} = \Theta^{\mu 3}$ and $\Theta^{\nu\mu} = \Theta^{\mu\nu}$. Interestingly, we reached the same conclusion from the first Bianchi-Padova relation. We will of course obtain a non-trivial consequence of the fourth Bianchi-Padova identity whenever $\alpha^{\mu k} \neq 0$.

The results of this section are summarized in Table 2. It is worth mentioning that most of these implications have not appeared previously in the context of defective structured surfaces.

3.2 The Induced Riemannian Structure

The coefficients L^i_{jk} of any general affine connection of a manifold $\mathcal{M}$, with non-trivial torsion ${\tilde{T}_{ij}}^p$ and non-metricity $\tilde{Q}_{kij}$, can be decomposed as [63, p. 141]

$$L^i_{jk} = \Gamma^i_{jk} + {\tilde{W}_{jk}}^{\;i}, \tag{34}$$

where the functions Γ^i_{jk} are coefficients of the Levi-Civita connection (torsion-free, metric-compatible) induced by the metric g_{ij}:

$$\Gamma^i_{jk} := \frac{1}{2} g^{ip}(g_{pk,j} + g_{pj,k} - g_{jk,p}), \tag{35}$$

with $[g^{ij}] := [g_{ij}]^{-1}$, and

$${\tilde{W}_{ij}}^{\;k} := {\tilde{C}_{ij}}^{\;k} + {\tilde{M}_{ij}}^{\;k}, \tag{36a}$$

$${\tilde{C}_{ij}}^{\;k} := g^{kp}\big(-\tilde{T}_{ipj} + \tilde{T}_{pji} - \tilde{T}_{jip}\big), \quad \text{and} \tag{36b}$$

$${\tilde{M}_{ij}}^{\;k} := \frac{1}{2} g^{kp}\big(\tilde{Q}_{ipj} - \tilde{Q}_{pji} + \tilde{Q}_{jip}\big). \tag{36c}$$

The functions ${\tilde{C}_{ij}}^{\;k}$ form the components of the contortion tensor, whereas the tensor ${\tilde{M}_{ij}}^{\;k}$ is an equivalent measure of non-metricity. The covariant components

$$\tilde{R}_{kljp} := g_{pi}\big(\Gamma^i_{lj,k} - \Gamma^i_{kj,l} + \Gamma^h_{lj}\Gamma^i_{kh} - \Gamma^h_{kj}\Gamma^i_{lh}\big) \tag{37}$$

of the Riemann–Christoffel curvature tensor of the Levi-Civita connection and the components $\tilde{\Omega}_{kljp}$ of the material curvature are related as [63, p. 141]

$$\tilde{R}_{ijpl} = \tilde{\Omega}_{ijpl} - 2\tilde{\partial}_{[i}\tilde{W}_{j]pl} - 2\tilde{W}_{[i|ml|}\tilde{W}_{j]p}{}^{m}, \tag{38}$$

where $\tilde{W}_{ijp} := \tilde{W}_{ij}{}^{k} g_{kp}$ and $\tilde{\partial}$ denotes covariant differentiation with respect to the Levi-Civita connection Γ. From the general symmetry relations, $\tilde{R}_{ijkl} = \tilde{R}_{klij} = -\tilde{R}_{jikl}$, of the Riemannian curvature induced by a metric, it is evident that it has only six independent components characterized by $\tilde{R}_{\alpha\beta\mu\nu}$, $\tilde{R}_{\alpha\beta\mu 3}$, and $\tilde{R}_{\alpha 3\beta 3}$. The only non-trivial relations out of (38), when restricted to $\zeta = 0$, are

$$R_{\alpha\beta\mu\nu} = \Omega_{\alpha\beta\mu\nu} - 2\partial_{[\alpha}W_{\beta]\mu\nu} - 2W_{[\alpha|i\nu|}W_{\beta]\mu}{}^{i}, \tag{39a}$$

$$R_{\alpha\beta\mu 3} = \Omega_{\alpha\beta\mu 3} - 2\partial_{[\alpha}W_{\beta]\mu 3} - 2W_{[\alpha|i3|}W_{\beta]\mu}{}^{i}, \quad \text{and} \tag{39b}$$

$$R_{\alpha 3\mu 3} = \Omega_{\alpha 3\mu 3} - \partial_{\alpha}W_{3\mu 3} - 2W_{[\alpha|i3|}W_{3]\mu}{}^{i}. \tag{39c}$$

Here, $R_{ijkl}(\theta^{\alpha}) := \tilde{R}_{ijkl}(\theta^{\alpha}, 0)$, $W_{ijk}(\theta^{\alpha}) := \tilde{W}_{ijk}(\theta^{\alpha}, 0)$, $W_{ij}{}^{k}(\theta^{\alpha}) := \tilde{W}_{ij}{}^{k}(\theta^{\alpha}, 0)$, and ∂ denotes covariant differentiation with respect to the projected Levi-Civita connection on U, consisting of components $s^{\mu}_{\alpha\beta} := \Gamma^{\mu}_{\alpha\beta}\big|_{\zeta=0}$. Therefore, for a differentiable tangent vector field $v_{\alpha}(\theta^{\beta})\boldsymbol{A}^{\alpha}$, $\partial_{\alpha}v_{\beta} := v_{\beta,\alpha} - s^{\mu}_{\alpha\beta}v_{\mu}$. The relations (39a)–(39c) are central to the theory of mechanics of defects as they are directly related to the strain incompatibility equations which we discuss next. Indeed, once we have identified the material metric $\boldsymbol{g}$ in terms of the strain fields associated with the structured surface, (39a)–(39c) constitute a system of PDEs for the strain fields, with defect densities as source terms. It should be noted that the components $\Omega_{\mu 3\alpha\beta}$ do not appear in any of (39a)–(39c). This is because, according to the fourth Bianchi-Padova relation (32), they can be written in terms of $\Omega_{\alpha\beta\mu 3}$ and other defect measures, and hence are not independent quantities.

4 Strain Incompatibility Relations for Structured Surfaces

In this section, we begin by introducing the notion of strain for a structured surface. The complete set of strains represent essentially the kinematical nature of shell theory that is being employed to describe structured surfaces. The strain fields also provide us with the fundamental variables for constructing the constitutive response functions associated with the continuum. Once the strain fields are fixed, we look for the necessary and sufficient (compatibility) conditions for the existence of a local isometric embedding of the surface in the 3-dimensional Euclidean space $\mathbb{R}^3$. The existence of such an isometric embedding is synonymous to the existence of a local sufficiently smooth bijective deformation map which is related to the given strain fields in a specified manner. Towards this end, we will construct the material metric $\boldsymbol{g}$ in the tubular neighbourhood $\mathcal{M}$ of $U \subset \omega$ using the strain fields given on U. The local compatibility then follows by requiring that the Riemannian space associated with $\boldsymbol{g}$ is flat, i.e., curvature free. Finally, we discuss how various defect densities become sources of strain incompatibility precluding the existence of the local isometric embedding. This will then set the stage for posing complete boundary-value-problems for stress distribution and natural shapes of defective structured surfaces, as will be discussed subsequently in Sect. 5. In the following we are only concerned with the local compatibility and incompatibility conditions, while providing their global counterpart elsewhere [57, 58].

4.1 Strain Measures and Strain Compatibility

Let us assume that there exist a local isometric embedding $\boldsymbol{R}: U \subset \omega \to \mathbb{R}^3$ of ω into $\mathbb{R}^3$. Let $\boldsymbol{A}_\alpha := \boldsymbol{R}_{,\alpha}$ and $\boldsymbol{N} := \boldsymbol{A}_1 \times \boldsymbol{A}_2/|\boldsymbol{A}_1 \times \boldsymbol{A}_2|$. The first and second fundamental forms associated with this embedding are therefore $A_{\alpha\beta} = \boldsymbol{A}_\alpha \cdot \boldsymbol{A}_\beta$ and $B_{\alpha\beta} = -\boldsymbol{N}_{,\beta} \cdot \boldsymbol{A}_\alpha$, respectively. We consider the following sufficiently smooth fields, defined over $\boldsymbol{R}(U)$, as descriptors of strain on the structured surface: (i) a symmetric tensor $E_{\alpha\beta}$, representing the in-surface strain field for measuring the local changes in length and angle; (ii) a tensor $\Lambda_{\alpha\beta}$ for transverse bending strains; (iii) two vectors Δ_α and Λ_α for measuring transverse shear and normal bending strains, respectively; and (iv) a scalar Δ for normal expansion/contraction. We now pose the central question for conditions of local strain compatibility.

Given sufficiently smooth strain fields (i)–(iv) over a fixed local isometric embedding $\boldsymbol{R}(U)$ of a 2-dimensional manifold ω, with first and second fundamental forms $A_{\alpha\beta}(\theta^\alpha)$ and $B_{\alpha\beta}(\theta^\alpha)$, respectively, what are the conditions to be satisfied for there to exist a sufficiently smooth local isometric embedding $\boldsymbol{r}: U \subset \omega \to \mathbb{R}^3$, with first and second fundamental forms $a_{\alpha\beta}$ and $b_{\alpha\beta}$ suitably constructed out of the given fields, along with a sufficiently smooth director field $\boldsymbol{d}: \boldsymbol{r}(U) \to \mathbb{R}^3$, so that the equations

$$E_{\alpha\beta} = \frac{1}{2}(\boldsymbol{a}_\alpha \cdot \boldsymbol{a}_\beta - \boldsymbol{A}_\alpha \cdot \boldsymbol{A}_\beta) = \frac{1}{2}(a_{\alpha\beta} - A_{\alpha\beta}), \tag{40a}$$

$$\Delta_\alpha = \boldsymbol{d} \cdot \boldsymbol{a}_\alpha - \boldsymbol{N} \cdot \boldsymbol{A}_\alpha = d_\alpha, \tag{40b}$$

$$\Delta = \boldsymbol{d} \cdot \boldsymbol{a}_3 - \boldsymbol{N} \cdot \boldsymbol{N} = d_3 - 1, \tag{40c}$$

$$\Lambda_{\alpha\beta} = \boldsymbol{d}_{,\beta} \cdot \boldsymbol{a}_\alpha - \boldsymbol{N}_{,\beta} \cdot \boldsymbol{A}_\alpha = \partial_\beta d_\alpha - d_3\, b_{\alpha\beta} + B_{\alpha\beta}, \quad \text{and} \tag{40d}$$

$$\Lambda_\beta = \boldsymbol{d}_{,\beta} \cdot \boldsymbol{a}_3 - \boldsymbol{N}_{,\beta} \cdot \boldsymbol{N} = d_{3,\beta} + d_\mu\, b^\mu_\beta, \tag{40e}$$

are satisfied on U such that $\boldsymbol{a}_\alpha := \boldsymbol{r}_{,\alpha}$, $\boldsymbol{a}_3 := \boldsymbol{a}_1 \times \boldsymbol{a}_2/|\boldsymbol{a}_1 \times \boldsymbol{a}_2|$? Here, recall that, ∂ is the covariant derivative with respect to the surface Christoffel symbols $s^\mu_{\alpha\beta}$, which are induced by the metric $a_{\alpha\beta}$ on the deformed base configuration. Clearly, the strain fields measure deformation of the structured surface from its reference configuration $(\boldsymbol{R}(U), \boldsymbol{N}(U))$ to the deformed configuration $(\boldsymbol{r}(U), \boldsymbol{d}(U))$. The necessary and sufficient conditions, to be satisfied by the given strain fields, so that a local deformed configuration of the structured surface does exist such that (40a)–(40e) are satisfied, are called local strain compatibility conditions. These are nothing but the integrability conditions for $\boldsymbol{r}$ and $\boldsymbol{d}$, as inferred from the system of PDEs in (40a)–(40e).

The *local strain compatibility conditions*, over a simply connected open set $W \subset U$, are given by

$$a_{\alpha\beta} := A_{\alpha\beta} + 2E_{\alpha\beta} \text{ is positive-definite}, \tag{41a}$$

$$\Delta \neq -1, \tag{41b}$$

$$\Lambda_\beta - \Delta_{,\beta} - \Delta_\mu b^\mu_\beta = 0, \tag{41c}$$

$$\Lambda_{[\alpha\beta]} - \partial_{[\beta}\Delta_{\alpha]} = 0, \tag{41d}$$

$$\partial_1 b_{21} - \partial_2 b_{11} = 0, \tag{41e}$$

$$\partial_1 b_{22} - \partial_2 b_{12} = 0, \quad \text{and} \tag{41f}$$

$$K_{1212} - \left(b_{12}^2 - b_{11}b_{22}\right) = 0, \tag{41g}$$

where

$$b_{\alpha\beta} := \frac{\partial_{(\beta}\Delta_{\alpha)} - \Lambda_{(\alpha\beta)} + B_{\alpha\beta}}{\Delta + 1} \tag{42}$$

is symmetric and K_{1212} is the only independent component of the Riemann–Christoffel curvature of the Levi-Civita connection on U induced by $a_{\alpha\beta}$. We assume $\Delta \neq -1$ for (42) to be a valid definition. This would physically mean that directors are nowhere tangential to the base surface (see Remark 1 for the situation otherwise). Equations (41e), (41f), and (41g) are the well-known Codazzi–Mainardi and Gauss equations for $a_{\alpha\beta}$ and $b_{\alpha\beta}$. Whenever these conditions are satisfied by the strain fields, there exists a sufficiently smooth local isometric embedding $\boldsymbol{r} : W \to \mathbb{R}^3$, with first and second fundamental form given by $a_{\alpha\beta}$ and $b_{\alpha\beta}$, respectively, and a director field $\boldsymbol{d} : \boldsymbol{r}(U) \to \mathbb{R}^3$ given by $d_\alpha = \Delta_\alpha$, $d_3 = \Delta + 1$, such that the PDEs (40a)–(40e) are identically satisfied everywhere on W. A strain field which does not satisfy all of the conditions (41a)–(41g) is called *incompatible*. The local strain compatibility conditions for the classical nonlinear shell theory, where $\Delta_\alpha = \Delta = \Lambda_\beta \equiv 0$, follow from (41e)–(41g) [11, 12, 35, 53]. The compatibility conditions for the single director Cosserat shell, as provided in (41a)–(41g), were derived by Epstein [20], cf. [44]. More general compatibility conditions for micropolar shells have been discussed by Zubov [73] and more recently by Eremeyev and Altenbach [22]. The following proof of the compatibility conditions is however based on our recent work [59]. The proof follows a methodology used by Ciarlet [12, Theorem 2.8-1] to establish compatibility conditions for the classical nonlinear shell. The nature of proof is central to our work since it directly leads us to the incompatibility equations in Sect. 4.2.

Assume the given strain fields $E_{\alpha\beta}$, $\Lambda_{\alpha\beta}$, Λ_α, Δ_α, and Δ to be sufficiently smooth on ω. The surface strain $E_{\alpha\beta}$ should be such that $a_{\alpha\beta}$, defined in (41a), is positive-definite so that it can qualify as a first fundamental form associated with ω. We construct a material metric $\boldsymbol{g}$ with components

$$g_{\alpha\beta} := a_{\alpha\beta} + \zeta\, P_{\alpha\beta} + \zeta^2\, Q_{\alpha\beta}, \qquad g_{\alpha 3} = g_{3\alpha} := \Delta_\alpha + \zeta\, U_\alpha, \qquad g_{33} := Z, \tag{43}$$

where

$$P_{\alpha\beta} := 2(\Lambda_{(\alpha\beta)} - B_{\alpha\beta}), \tag{44a}$$

$$Q_{\alpha\beta} := a^{\sigma\gamma}\,(\Lambda_{\sigma\alpha} - B_{\sigma\alpha})(\Lambda_{\gamma\beta} - B_{\gamma\beta}) + \Lambda_\alpha\,\Lambda_\beta, \tag{44b}$$

$$U_\alpha := a^{\sigma\gamma}\,\Delta_\sigma(\Lambda_{\gamma\alpha} - B_{\gamma\alpha}) + \Lambda_\alpha(\Delta + 1), \quad \text{and} \tag{44c}$$

$$Z := a^{\alpha\beta}\,\Delta_\alpha\Delta_\beta + (\Delta + 1)^2. \tag{44d}$$

In the above, $[a^{\alpha\beta}] := [a_{\alpha\beta}]^{-1}$. Note that, since U is bounded and g_{ij} is continuous in θ^α and ζ, g_{ij} will be positive-definite on $V := U \times (-\epsilon, \epsilon) \subset \mathcal{M}$ for sufficiently small ϵ. Our result is valid for this sufficiently small ϵ and we *a priori* construct $\mathcal{M}$ such that ϵ conforms to this small value throughout. For a technical discussion on the issue of smallness of ϵ and positive definiteness of g_{ij}, refer to the proof of Theorem 2.8-1 in [12]. The 'sufficient thinness' of the structured surface is encoded in the definition (43) which describes how the 2-dimensional strain fields can be used to construct a 3-dimensional metric over the tubular neighbourhood $\mathcal{M}$ of ω. The parameter ϵ can be thought of as a physical length scale inherent to the description of the structured surface, e.g., thickness of a shell structure or the length of the individual molecules (not necessarily transverse to the surface) in lipid membranes. The 3-dimensional metric $\boldsymbol{g}$ is of second-order in the transverse coordinate ζ

and this dependence brings out the non-locality of the director gradient in the kinematics of the structured surface, taking into account the transverse shear and normal distortion of the attached directors. The form of the metric in (43) is a generalization of the metric with components

$$g_{\alpha\beta}(\theta^\alpha, \zeta) = a_{\alpha\beta} - 2\zeta b_{\alpha\beta} + \zeta^2 a^{\mu\nu} b_{\mu\alpha} b_{\nu\beta}, \qquad g_{\alpha 3} = g_{3\alpha} = 0, \qquad g_{33} = 1. \tag{45}$$

This form appeared in the seminal paper on nonlinear shell theory by Koiter [35], where the kinematics was otherwise assumed to be of the Kirchhoff–Love type (i.e., $\Lambda_\alpha = \Delta_\alpha = \Delta = 0$). In the above equation, $b_{\alpha\beta} = -\Lambda_{(\alpha\beta)} + B_{\alpha\beta}$, and hence any normal distortion or transverse shearing of the directors is ignored.

The coefficients of the Levi-Civita connection of the metric (43), defined by $\Gamma^q_{ij} := g^{pq}\Gamma_{ijp}$ where $\Gamma_{ijp} := \frac{1}{2}(g_{ip,j} + g_{jp,i} - g_{ij,p})$, can be calculated by noting that

$$\Gamma_{333} = 0, \qquad \Gamma_{33\rho} = U_\rho - \frac{1}{2} Z_{,\rho}, \qquad \Gamma_{3\rho 3} = \Gamma_{\rho 33} = \frac{1}{2} Z_{,\rho}, \tag{46a}$$

$$\Gamma_{3\rho\sigma} = \Gamma_{\rho 3\sigma} = \Delta_{[\sigma,\rho]} + \frac{1}{2} P_{\rho\sigma} + \zeta\, (U_{[\sigma,\rho]} + Q_{\rho\sigma}), \tag{46b}$$

$$\Gamma_{\rho\sigma 3} = \Delta_{(\sigma,\rho)} - \frac{1}{2} P_{\rho\sigma} + \zeta\, (U_{(\sigma,\rho)} - Q_{\rho\sigma}), \quad \text{and} \tag{46c}$$

$$\Gamma_{\rho\sigma\delta} = s_{\rho\sigma\delta} + \frac{\zeta}{2}(P_{\rho\delta,\sigma} + P_{\sigma\delta,\rho} - P_{\sigma\rho,\delta}) + \frac{\zeta^2}{2}(Q_{\rho\delta,\sigma} + Q_{\sigma\delta,\rho} - Q_{\sigma\rho,\delta}), \tag{46d}$$

where $s_{\rho\sigma\delta} := \frac{1}{2}(a_{\rho\delta,\sigma} + a_{\sigma\delta,\rho} - a_{\rho\sigma,\delta})$. The local strain compatibility conditions are the conditions for the embedding space $\mathcal{M}$ to be Euclidean, i.e., the Riemann–Christoffel curvature $\tilde{R}_{ijkl}$ of the metric (43) to become identically zero. However, as shown elsewhere [59], in order to ensure compatibility of the 2-dimensional strain fields, it is enough to impose that $\tilde{R}_{ijkl}\big|_{\zeta=0} = R_{ijkl}(\theta^\alpha) = 0$. The curvature R_{ijkl} has six independent components such that $R_{ijkl} = 0$ if and only if $R_{1212} = 0$, $R_{12\sigma 3} = 0$, and $R_{\rho 3\sigma 3} = 0$. After some manipulation, it can be shown that

$$R_{1212} = K_{1212} - \left(b_{12}^2 - b_{11} b_{22}\right), \tag{47}$$

where the functions $K_{\beta\alpha\mu\nu} := a_{\rho\nu}(s^\rho_{\alpha\mu,\beta} - s^\rho_{\beta\mu,\alpha} + s^\delta_{\alpha\mu} s^\rho_{\beta\delta} - s^\delta_{\beta\mu} s^\rho_{\alpha\delta})$ constitute the covariant components of the Riemann–Christoffel curvature of the surface Levi-Civita connection $s^\mu_{\alpha\nu} = a^{\mu\rho} s_{\alpha\nu\rho}$. These, by definition, have the symmetries $K_{\alpha\beta\mu\nu} = -K_{\alpha\beta\nu\mu} = K_{\mu\nu\alpha\beta}$ and, hence, have only one independent component $K := \frac{1}{4}\varepsilon^{\alpha\beta}\varepsilon^{\mu\nu} K_{\alpha\beta\mu\nu}$, the Gaussian curvature induced by the surface metric $a_{\alpha\beta}$, where $\varepsilon^{\alpha\beta} := a^{-\frac{1}{2}} e^{\alpha\beta}$ ($e^{\alpha\beta} = e_{\alpha\beta}$ is the 2-dimensional permutation symbol) and $a := \det[a_{\alpha\beta}]$. It is easily seen that $K_{1212} = 4aK$. Consequently, $R_{1212} = 0$, in conjunction with (47), can be used to infer (41g), which is the single independent Gauss equation satisfied by $a_{\alpha\beta}$ and $b_{\alpha\beta}$. Further, we can evaluate

$$R_{1213} = a^{2\beta}\Delta_\beta\left(K_{2121} - \left(b_{12}^2 - b_{11} b_{22}\right)\right) - (\Delta + 1)(\partial_2 b_{11} - \partial_1 b_{12}) \quad \text{and} \tag{48}$$

$$R_{1223} = -a^{1\beta}\Delta_\beta\left(K_{1212} - \left(b_{12}^2 - b_{11} b_{22}\right)\right) - (\Delta + 1)(\partial_2 b_{21} - \partial_1 b_{22}). \tag{49}$$

Substituting (41g) in (48) and (49), the condition $R_{12\sigma 3} = 0$ yields (41e) and (41f), which are the two independent Codazzi–Mainardi equations satisfied by $a_{\alpha\beta}$ and $b_{\alpha\beta}$. The Gauss and Codazzi–Mainardi equations satisfied over a simply connected domain $W \subset U$ ensure the existence of a local isometric embedding $\boldsymbol{r}: W \to \mathbb{R}^3$, with first fundamental form $a_{\alpha\beta}$ and second fundamental form $b_{\alpha\beta}$, modulo isometries of $\mathbb{R}^3$. Finally, we calculate

$$R_{\rho 3\sigma 3} = (\Delta+1)\,\partial_{(\sigma} I_{\rho)} - \Lambda_{(\rho} I_{\sigma)} - a^{\alpha\beta}\Delta_\alpha \left\{ b_{\beta(\rho} I_{\sigma)} + \frac{1}{2} e_{\beta(\rho} I_{\sigma)} J - b_{\rho\sigma} I_\beta \right\} + \left(a^{\alpha\beta}(\Delta+1)^2 + a^{\alpha\mu}a^{\beta\nu}\Delta_\mu\Delta_\nu\right)(J)^2 e_{\alpha\rho} e_{\beta\sigma}, \tag{50}$$

where

$$I_\beta := \Lambda_\beta - \Delta_{,\beta} - \Delta_\alpha a^{\alpha\gamma} b_{\gamma\beta} \quad \text{and} \quad J := \frac{\varepsilon^{\alpha\beta}\left(\partial_{[\beta}\Delta_{\alpha]} - \Lambda_{[\alpha\beta]}\right)}{2(\Delta+1)}. \tag{51}$$

The condition $R_{\rho 3\sigma 3} = 0$ is a set of three coupled first-order homogeneous non-linear partial differential algebraic equations for three unknowns I_α and J. It has been argued elsewhere [59] that the only physically meaningful solution of these equations is the trivial set $I_\alpha = 0$ and $J = 0$; the non-zero solutions become unstable under generic perturbations of the zero solution set. These equalities are equivalent to (41c) and (41d), respectively. They ensure the existence of a well-defined director field $\boldsymbol{d}: \boldsymbol{r}(W) \to \mathbb{R}^3$, defined by $d_\alpha = \Delta_\alpha$ and $d_3 = \Delta + 1$ (see (40b) and (40c)), which satisfies (40d) and (40e) identically over any simply connected open set $W \subset \omega$. This finishes our proof.

Remark 1 (Structured surfaces with tangential director field) When the director fields are everywhere tangential to their respective base surfaces, we choose the reference director field $\boldsymbol{D}$ to be some known tangent vector field over $\boldsymbol{R}(\omega)$ (rather than the normal field $\boldsymbol{N}$). The relations (40a)–(40e) are replaced by

$$E_{\alpha\beta} = \frac{1}{2}(\boldsymbol{a}_\alpha \cdot \boldsymbol{a}_\beta - \boldsymbol{A}_\alpha \cdot \boldsymbol{A}_\beta) = \frac{1}{2}(a_{\alpha\beta} - A_{\alpha\beta}), \tag{52a}$$

$$\Delta_\alpha = \boldsymbol{d} \cdot \boldsymbol{a}_\alpha - \boldsymbol{D} \cdot \boldsymbol{A}_\alpha = d_\alpha - D_\alpha, \tag{52b}$$

$$\Lambda_{\alpha\beta} = \boldsymbol{d}_{,\beta} \cdot \boldsymbol{a}_\alpha - \boldsymbol{D}_{,\beta} \cdot \boldsymbol{A}_\alpha = \partial_\beta d_\alpha - \bar{\partial}_\beta D_\alpha, \quad \text{and} \tag{52c}$$

$$\Lambda_\beta = \boldsymbol{d}_{,\beta} \cdot \boldsymbol{n} - \boldsymbol{D}_{,\beta} \cdot \boldsymbol{N} = d_\mu b^\mu_\beta - D_\mu B^\mu_\beta, \tag{52d}$$

where $\bar{\partial}$ denotes the covariant derivative with respect to the induced Levi-Civita connection $\bar{s}^\mu_{\alpha\beta}$ by the metric $A_{\alpha\beta}$ on the reference embedding $\boldsymbol{R}(\omega)$, hence for a differentiable tangent vector field $\boldsymbol{v}$, $\bar{\partial}_\alpha v_\beta := v_{\beta,\alpha} - \bar{s}^\mu_{\alpha\beta} v_\mu$. The integrability conditions for the above PDEs, for unknown $\boldsymbol{r}$ and $\boldsymbol{d}$, given $A_{\alpha\beta}$, $B_{\alpha\beta}$, D_α, and the strain fields, provide the local strain compatibility conditions. To derive local compatibility relations, we note that the metric of the deformed surface is completely determined by (52a), $a_{\alpha\beta} := A_{\alpha\beta} + 2E_{\alpha\beta}$, with $E_{\alpha\beta}$ such that $a_{\alpha\beta}$ is positive-definite; this is same as before. However, we no longer have a straight forward formula for the functions $b_{\alpha\beta}$. As a candidate for the second fundamental form of the deformed surface, we choose any $b_{\alpha\beta}$ that solves the algebraic equation

$$(\Delta_\mu + D_\mu) b^\mu_\beta = \Lambda_\beta + D_\mu B^\mu_\beta, \tag{53}$$

which is arrived after eliminating d_α between (52b) and (52d). The Codazzi–Mainardi and Gauss equations involving $a_{\alpha\beta}$ and $b_{\alpha\beta}$ provide the first set of strain compatibility conditions, ensuring the existence of a local embedding $\boldsymbol{r}: W \subset U \to \mathbb{R}^3$, for a simple connected W, with first and second fundamental forms given by $a_{\alpha\beta}$ and $b_{\alpha\beta}$, respectively, modulo isometries of $\mathbb{R}^3$. The other strain compatibility condition is given by

$$\Lambda_{\alpha\beta} = \partial_\beta(\Delta_\alpha + D_\alpha) - \bar{\partial}_\beta D_\alpha, \tag{54}$$

obtained by eliminating d_α between (52b) and (52c). This ensures the existence of a tangential director field $\boldsymbol{d} : \boldsymbol{r}(W) \to \mathbb{R}^3$ such that (52a)–(52d) are satisfied. To the best of our knowledge, the above compatibility conditions have not appeared elsewhere.

4.2 Strain Incompatibility Arising from Defects

It is well-known that distributed defects within the material structure are inherent sources of strain incompatibility and, hence, residual stress [13, 38, 39]. The loss of local strain compatibility is tantamount to the non-existence of a local deformation map from a given connected subset of Euclidean space. In the context of structured surfaces, this means that the fields $a_{\alpha\beta}$ and $b_{\alpha\beta}$, constructed out of an incompatible strain using (41a) and (42), do not correspond to the first and second fundamental form of any realizable isometric embedding of ω into $\mathbb{R}^3$, not even locally. At least some of the strain compatibility conditions must be violated in the presence of defects. Indeed, according to (39a)–(39c), the curvature R_{ijkl} associated with the metric no longer vanishes when the defect densities are non-trivial. There remains a possibility of non-zero defect distributions such that the right-hand-sides of (39a)–(39c) vanish all together. In such cases, material defects no longer act as sources of strain incompatibility. The local *strain incompatibility relations* can be obtained by combining (39a)–(39c) with the expressions (47)–(50). The resulting relations are non-linear inhomogeneous partial differential equations for the strain fields with the source terms in the form of various defect densities. They are collected below:

$$K_{1212} - \left[b_{12}^2 - b_{11}b_{22}\right] = g\Theta^3 - 2\partial_{[1}W_{2]12} - 2W_{[1|i2|}W_{2]1}{}^i, \tag{55}$$

$$\begin{aligned} &a^{2\beta}\Delta_\beta\left(K_{1212} - \left[b_{12}^2 - b_{11}b_{22}\right]\right) - (\Delta+1)[\partial_2 b_{11} - \partial_1 b_{12}] \\ &\quad = -g\Theta^2 - 2\partial_{[1}W_{2]13} - 2W_{[1|i3|}W_{2]1}{}^i, \end{aligned} \tag{56}$$

$$\begin{aligned} &-a^{1\beta}\Delta_\beta\left(K_{1212} - \left[b_{12}^2 - b_{11}b_{22}\right]\right) - (\Delta+1)[\partial_2 b_{21} - \partial_1 b_{22}] \\ &\quad = g\Theta^1 - 2\partial_{[1}W_{2]23} - 2W_{[1|i3|}W_{2]2}{}^i, \quad \text{and} \end{aligned} \tag{57}$$

$$\begin{aligned} &(\Delta+1)\,\partial_{(\sigma}I_{\rho)} - \Lambda_{(\rho}I_{\sigma)} - a^{\alpha\beta}\Delta_\alpha\left\{b_{\beta(\rho}I_{\sigma)} + \frac{1}{2}e_{\beta(\rho}I_{\sigma)}J - b_{\rho\sigma}I_\beta\right\} \\ &\qquad + \left(a^{\alpha\beta}(\Delta+1)^2 + a^{\alpha\mu}a^{\beta\nu}\Delta_\mu\Delta_\nu\right)(J)^2\varepsilon_{\alpha\rho}\varepsilon_{\beta\sigma} \\ &\quad = \varepsilon_{\rho3\nu}\varepsilon_{\sigma3\mu}\Theta^{\nu\mu} - \partial_\rho W_{3\sigma3} - 2W_{[\rho|i3|}W_{3]\sigma}{}^i. \end{aligned} \tag{58}$$

These local strain incompatibility relations are written for a continuously defective structured surface in their full generality. We recall, from Sect. 3.2, that the functions $W_{ij}{}^k$ are defined in terms of dislocation densities and metric anomalies as $W_{ij}{}^k = C_{ij}{}^k + M_{ij}{}^k$, where the components $C_{ij}{}^k$ of contortion tensor are algebraic functions of the dislocation densities J^i and $\alpha^{\mu k}$, and the components $M_{ij}{}^k$ are algebraic functions of the densities of metric anomalies Q_{kij}, see (36a)–(36c). In the absence of dislocations and metric anomalies, i.e., when $W_{ij}{}^k \equiv 0$, clearly, the density of wedge disclinations Θ^3 act as the single source to the incompatibility of the Gauss equation (55), while the densities of twist disclinations/intrinsic orientational anomalies $\Theta^{\mu} = \Theta^{\mu 3}$ are the only source terms to the incompatible Codazzi–Mainardi equations (56) and (57); the symmetric disclination density fields $\Theta^{\mu\nu}$ are sources to non-trivial I_α and J. Note that, the disclination densities $\Theta^{\mu 3}$ seem to be absent from the above relations. This is so because they are not independent but expressible in terms of Θ^{μ} and other defect densities as a consequence of the fourth Bianchi-Padova relation.

The local strain incompatibility relations for classical nonlinear shell with Kirchhoff–Love kinematics can be easily deduced from the above relations. The material metric now has a simple block diagonal form, given in (45), such that $\Delta = \Delta_\alpha = \Lambda_\alpha = 0$. Also, from (51), we can infer that $I_\alpha = 0$ and $J = -(1/2)\varepsilon^{\alpha\beta}\Lambda_{[\alpha\beta]}$. The incompatibility relations then reduce to

$$K_{1212} - \left[b_{12}^2 - b_{11}b_{22}\right] = a\Theta^3 - 2\partial_{[1} W_{2]12} - 2W_{[1|i2|} W_{2]1}{}^{i}, \tag{59}$$

$$-\partial_2 b_{11} + \partial_1 b_{12} = -a\Theta^2 - 2\partial_{[1} W_{2]13} - 2W_{[1|i3|} W_{2]1}{}^{i}, \tag{60}$$

$$-\partial_2 b_{21} + \partial_1 b_{22} = a\Theta^1 - 2\partial_{[1} W_{2]23} - 2W_{[1|i3|} W_{2]2}{}^{i}, \quad \text{and} \tag{61}$$

$$a^{\alpha\beta}(\Lambda_{[\alpha\beta]})^2\varepsilon_{\alpha\rho}\varepsilon_{\beta\sigma} = \varepsilon_{\rho\nu}\varepsilon_{\sigma\mu}\Theta^{\nu\mu} - \partial_\rho W_{3\sigma 3} - 2W_{[\rho|i3|} W_{3]\sigma}{}^{i}. \tag{62}$$

In many applications, to follow in the next section, we will restrict attention to sufficiently thin structured surfaces, e.g., 2-dimensional crystals, purely disclinated nematic membranes, monolayer bio-membranes, etc. In such cases the $\Theta^{\mu\nu}$-disclinations and $\alpha^{\mu k}$-dislocations are naturally absent. We will additionally make realistic assumptions on the smallness/vanishing of strain fields and defect densities and simplify equations (59)–(62) in Sect. 5.2. In particular, we will obtain specialized forms of the simplified relations that have already appeared in the literature.

5 Residual Stress and Natural Shapes

A central problem in the mechanics of solids is, for a given distribution of material defects, to determine the stress field and the deformed shape of the defective body with respect to a fixed reference configuration. The notion of defects is to be understood in the sense of material anomalies, as discussed in Sect. 2, which lead to an inhomogeneous material response in an otherwise materially uniform body. In particular, if we assume stress to be purely elastic in origin, then, in general, there is no one-to-one mapping from the current configuration of the defective body, which is realized as a connected set in the physical space, to its natural stress-free state. This means that the natural state of the defective material body cannot be realized as a connected set in the physical space. It also entails an incompatible *elastic strain field*, which appears as the energetic dual of stress, with sources of incompatibility derived from various defect densities. The absence of an elastic deformation map implies that there is no one-to-one map which connects the reference configuration to the natural state. The strain field which relates the natural configuration to the fixed reference configuration is termed *plastic strain*. It is called plastic because a change in the natural state can occur only due to defect evolution leading to irreversible changes in the material structure [39]. The plastic strains satisfy the incompatibility equations (55)–(58). The elastic strains will satisfy a different form of incompatibility equations with the reference configuration replaced by current configuration in the derivation of these equations. For this difference, they are more difficult to deal with since the current configuration is itself unknown. The plastic strain incompatibility relations are combined with the constitutive laws (relating elastic strains with stresses and moments), the equilibrium equations, and the boundary conditions to yield the full boundary-value-problem for the determination of stress field and natural shape of the structured surface for a given distribution of defects. A prescription, on how the strain fields—total, elastic, and plastic—are all related to each other, is also required.

The problem of relating the three configurations (reference, natural, and current) is usually addressed by assuming a multiplicative decomposition of the total distortion tensor into elastic and plastic distortion tensors. The total distortion tensor is the derivative map of the total deformation mapping (a bijective map between the reference and the current configuration) and hence yields a compatible total strain tensor. The elastic and plastic distortion tensors map tangent spaces from the natural configuration to the current configuration and from the reference configuration to the natural configuration, respectively. However, in the presence of disclination density, the elastic and plastic distortion tensors are not well-defined [59]. The ambiguity arises due to the rotational part of the tensors becoming multi-valued. Nevertheless, the multiplicative decomposition can be used for isotropic materials where both elastic and plastic rotations do not play any role in the final boundary-value-problem [14]. The need for a multiplicative decomposition can be circumnavigated if we assume an additive decomposition of the total strain into elastic and plastic counterparts. In such a situation, we do not require the notion of elastic and plastic distortion tensors at all. For 3-dimensional elastic solids, the additive decomposition of strain is essentially based on the smallness of both deformation and plastic strain (to the same order). The resulting theory is necessarily applicable to small deformation problems [15, 39]. On the other hand, an additive decomposition of strains, as proposed in Sect. 5.1, with the notion of strain, as defined in the beginning of Sect. 4.1 in the context of 2-dimensional structured surfaces, is less restrictive. It in fact allows for moderately large rotations in the deformation while maintaining small surface strains. This is important for structured surfaces since, unlike 3-dimensional bodies, they are very much likely to accommodate residual stresses by escaping into the third dimension via moderately large rotations. The nature of the assumed additive decomposition, which allows for a separation of order of the in-surface stretching and the bending modes of deformation for structured surfaces, will be discussed in detail in Sect. 5.1.

The kinematical assumptions on strain from Sect. 5.1, appended with certain smallness assumptions on the defect densities, are used in Sect. 5.2 to obtain a simplified form of strain incompatibility relations written for plastic strain. These relations are valid for Kirchhoff–Love shells with small surface strains but moderately large rotations. In Sect. 5.3, the plastic strain incompatibility conditions are combined with the equilibrium equations and constitutive functions of the classical Föppl–von Kármán shell theory to obtain a coupled system of partial differential equations to determine stress and deformed shape for a given distribution of defects and metric anomalies. Several applications are mentioned from the varied contexts of 2-dimensional solid crystals, growing biological surfaces, and isotropic fluid films. In particular, we point out connections of our theory with the existing work wherever possible.

5.1 Kinematics of Kirchhoff–Love Shells with Small Surface Strain Accompanied by Moderate Rotation

Following Sect. 4.1, we consider the fixed reference configuration of the Kirchhoff–Love structured surface to be given by a local isometric embedding $\boldsymbol{R} : U \to \mathbb{R}^3$, where U is a simply connected open set of ω; also, as before, we take (θ^α, ζ) as the adapted coordinates on U. The tangent spaces of $\boldsymbol{R}(U)$ are spanned by the natural basis vectors $\boldsymbol{A}_\alpha = \boldsymbol{R}_{,\alpha}$.

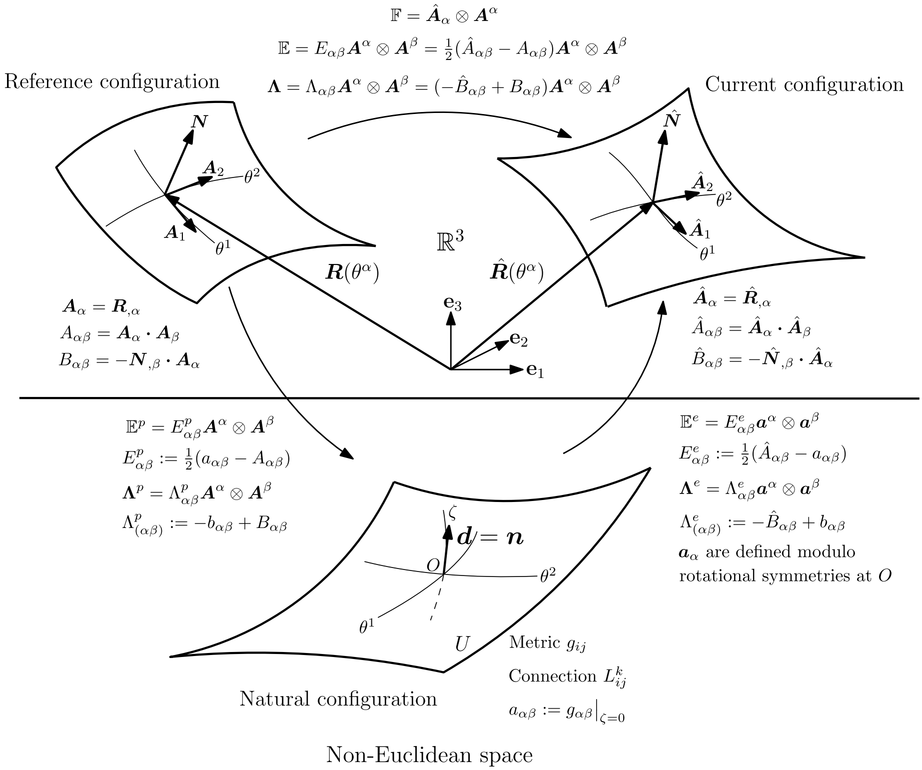


Fig. 8 Kinematics of the elastic-plastic decomposition of the total deformation measures in Kirchhoff–Love shells. The only non-trivial disclinations are represented by Θ^3, and hence we have a well defined normal over the surface in the natural configuration. The maps depicted in the figure are only for a local neighborhood of the structured surface

The first and second fundamental forms associated with the reference surface are given by $A_{\alpha\beta} = \boldsymbol{A}_\alpha \cdot \boldsymbol{A}_\beta$ and $B_{\alpha\beta} = -\boldsymbol{N}_{,\alpha} \cdot \boldsymbol{A}_\beta$, respectively, where $\boldsymbol{N} := \boldsymbol{A}_1 \times \boldsymbol{A}_2/|\boldsymbol{A}_1 \times \boldsymbol{A}_2|$ is the local unit normal. We will assume the adapted coordinates (θ^α, ζ) to be convected by deformation of the surface. The natural basis vectors $\hat{\boldsymbol{A}}_\alpha$ on the tangent spaces of the current configuration $\hat{\boldsymbol{R}} : U \to \mathbb{R}^3$, a different isometric embedding of U, are given by $\hat{\boldsymbol{A}}_\alpha = \hat{\boldsymbol{R}}_{,\alpha}$. The first and second fundamental forms associated with the current configuration are $\hat{A}_{\alpha\beta} = \hat{\boldsymbol{A}}_\alpha \cdot \hat{\boldsymbol{A}}_\beta$ and $\hat{B}_{\alpha\beta} = -\hat{\boldsymbol{N}}_{,\alpha} \cdot \hat{\boldsymbol{A}}_\beta$, respectively, where $\hat{\boldsymbol{N}} := \hat{\boldsymbol{A}}_1 \times \hat{\boldsymbol{A}}_2/|\hat{\boldsymbol{A}}_1 \times \hat{\boldsymbol{A}}_2|$. The reference and the current configurations are shown in Fig. 8. The pairs $(A_{\alpha\beta}, B_{\alpha\beta})$ and $(\hat{A}_{\alpha\beta}, \hat{B}_{\alpha\beta})$ individually satisfy the Gauss and Codazzi–Mainardi equations owing to the existence of isometric embeddings $\boldsymbol{R}$ and $\hat{\boldsymbol{R}}$. The total surface distortion tensor $\mathbb{F}$, which is the surface derivative map of the deformation mapping, relates the tangent spaces of $\boldsymbol{R}(U)$ to those of $\hat{\boldsymbol{R}}(U)$ such that $\mathbb{F} = \hat{\boldsymbol{A}}_\alpha \otimes \boldsymbol{A}^\alpha$. The total surface strain and the total bending strain tensors, defined as $\mathbb{E} = E_{\alpha\beta}\boldsymbol{A}^\alpha \otimes \boldsymbol{A}^\beta = \frac{1}{2}(\hat{A}_{\alpha\beta} - A_{\alpha\beta})\boldsymbol{A}^\alpha \otimes \boldsymbol{A}^\beta$ and $\boldsymbol{\Lambda} = \Lambda_{\alpha\beta}\boldsymbol{A}^\alpha \otimes \boldsymbol{A}^\beta = (-\hat{B}_{\alpha\beta} + B_{\alpha\beta})\boldsymbol{A}^\alpha \otimes \boldsymbol{A}^\beta$, respectively, measure the relative first and second fundamental forms of the current configuration with respect to the reference configuration of the structured surface. Other strain measures, introduced in the beginning of Sect. 4.1, are identically zero under the Kirchhoff–Love constraint (which imposes the director field to coincide with the unit normal field).

The elastic surface strain tensor $\mathbb{E}^e$ and the elastic bending strain tensor $\boldsymbol{\Lambda}^e$ are defined as energetic dual of the surface stress and bending moment tensors, respectively, see Sect. 5.3. On the other hand, the plastic surface strain and the plastic bending strain tensors are defined as $\mathbb{E}^p = E^p_{\alpha\beta}\boldsymbol{A}^\alpha \otimes \boldsymbol{A}^\beta$ and $\boldsymbol{\Lambda}^p = \Lambda^p_{\alpha\beta}\boldsymbol{A}^\alpha \otimes \boldsymbol{A}^\beta$, respectively, where $E^p_{\alpha\beta} := \frac{1}{2}(a_{\alpha\beta} - A_{\alpha\beta})$ and $\Lambda^p_{(\alpha\beta)} := -b_{\alpha\beta} + B_{\alpha\beta}$ such that $a_{\alpha\beta}$ and $b_{\alpha\beta}$ are, respectively, the first and second fundamental forms of U in the natural configuration. Here, and henceforth, we will use superscripts e and p to denote elastic and plastic variables, respectively (they should not be read as indices). We note that it is only in the absence of disclinations and intrinsic orientational anomalies that there exist well-defined crystallographic vector fields $\boldsymbol{a}_\alpha := \mathbb{F}^p \boldsymbol{A}_\alpha$ over the tangent spaces of local natural configuration U, where $\mathbb{F}^p$ is the (single-valued) plastic distortion field [59] (see Remark 2 for details). The elastic strain tensors can then be written as $\mathbb{E}^e = E^e_{\alpha\beta}\boldsymbol{a}^\alpha \otimes \boldsymbol{a}^\beta$ and $\boldsymbol{\Lambda}^e = \Lambda^e_{\alpha\beta}\boldsymbol{a}^\alpha \otimes \boldsymbol{a}^\beta$, where $E^e_{\alpha\beta} := \frac{1}{2}(\hat{A}_{\alpha\beta} - a_{\alpha\beta})$ and $\Lambda^e_{(\alpha\beta)} := -\hat{B}_{\alpha\beta} + b_{\alpha\beta}$ such that $\boldsymbol{a}^\alpha := a^{\alpha\beta}\boldsymbol{a}_\beta$ are the dual crystallographic vector fields on the material space. On the other hand, if the only non-trivial disclinations present are those modelled by Θ^3 (in-surface wedge disclinations) then the crystallographic vector fields $\boldsymbol{a}_\alpha$ are well-defined modulo rotation symmetries of the material surface with normal as the axis of rotation. In other words, the rotation part of the plastic distortion field (see Remark 2) is well-defined modulo the known rotations from the material symmetry group. The normal $\boldsymbol{n}$ at each point in the natural configuration is also well-defined in such a scenario, see Fig. 8. In rest of the paper, we will restrict our attention to this special case.

We now discuss the additive decomposition of the total strain tensor into elastic and plastic parts. Introduce a small parameter $\epsilon := h/R$, where h is the maximum thickness of the structured surface and R is the minimum radius of curvature that U can assume in all possible deformations. Let $\mathbb{E}$, $\mathbb{E}^p$, $\mathbb{E}^e$, and their first and second spatial derivatives be $O(\epsilon)$, and $\boldsymbol{\Lambda}$, $\boldsymbol{\Lambda}^p$, $\boldsymbol{\Lambda}^e$, and their first spatial derivatives be $O(\epsilon^{\frac{1}{2}})$. Here, following Landau's notation, for $\boldsymbol{f}: \mathbb{R} \to \mathbb{R}^k$, we write $\boldsymbol{f}(s) = O(s^r)$ if and only if there exist positive constants M and δ such that $||\boldsymbol{f}(s)||_{\mathbb{R}^k} \leq M|s|^r$ for all $|s| < \delta$, where r is any real number. Following Naghdi and Vongsarnpigoon [50], we emphasize that the resulting theory, where the surface and bending strains follow these separated orders, allows for *small surface strain accompanied by moderate rotation*. It can be shown that the total deformation is $O(\epsilon^{\frac{1}{2}})$ and is therefore more general than what is afforded by the geometrically linear shell theories. We postulate that the following decompositions for the total surface and bending strains hold:

$$\mathbb{E} = \mathbb{E}^e + \mathbb{E}^p \quad \text{and} \tag{63a}$$

$$\boldsymbol{\Lambda} = \boldsymbol{\Lambda}^e + \boldsymbol{\Lambda}^p. \tag{63b}$$

The first decomposition, which is $O(\epsilon)$, is the standard additive decomposition for small strains used commonly in small deformation theories. The second decomposition, which is $O(\epsilon^{\frac{1}{2}})$, is non-standard. Also, as $\boldsymbol{A}_\alpha = \hat{\boldsymbol{A}}_\alpha = \boldsymbol{a}_\alpha$ upto $O(\epsilon^{\frac{1}{2}})$, where in deriving the second equality we have used the fact that the symmetry rotations are $O(1)$, we have

$$E_{\alpha\beta} = E^e_{\alpha\beta} + E^p_{\alpha\beta} \quad \text{and} \tag{64a}$$

$$\Lambda_{\alpha\beta} = \Lambda^e_{\alpha\beta} + \Lambda^p_{\alpha\beta}. \tag{64b}$$

Note that, as $\Lambda_{\alpha\beta}$ is symmetric, necessarily $\Lambda^p_{[\alpha\beta]} = -\Lambda^e_{[\alpha\beta]}$. These approximated decompositions with the mentioned order hold for sufficiently thin structured surfaces where the bending mode dominates over surface stretching for a given internal or external loading.

Remark 2 Whenever disclinations and metric anomalies are identically absent, the material connection and material metric can be written as

$$L_{ij}^k = \left(F^{p^{-1}}\right)^{kq} F_{qi,j}^p \quad \text{and} \quad \boldsymbol{g} = \mathbf{F}^{p^T}\mathbf{F}^p \tag{65}$$

in terms of an invertible second-order tensor field $\mathbf{F}^p := F_{ij}^p \boldsymbol{G}^i \otimes \boldsymbol{G}^j$, the plastic distortion field, defined over simply connected subsets $V \subset \mathcal{M}$ [60]. The well-defined surface plastic distortion tensor $\mathbb{F}^p := \mathbf{F}^p\big|_{\zeta=0}$ maps the reference base vectors $\boldsymbol{A}_\alpha$ to the crystallographic base vectors $\boldsymbol{a}_\alpha := \mathbb{F}^p \boldsymbol{A}_\alpha$ over the material space. The plastic rotation in the polar decomposition $\mathbb{F}^p = \mathbb{R}^p\mathbb{U}^p$, where $\mathbb{U}^p$ $(= (\mathbf{1} + \mathbb{E}^p)^{1/2})$, with $\mathbf{1}$ being the 3-dimensional identity tensor) is the in-surface plastic stretch, is derivable by solving a first-order PDE involving the in-surface plastic strain [65]. Let $\boldsymbol{a}^\alpha := a^{\alpha\beta}\boldsymbol{a}_\beta$ be the dual crystallographic base vectors, $\boldsymbol{n} := \boldsymbol{a}_1 \times \boldsymbol{a}_2 / |\boldsymbol{a}_1 \times \boldsymbol{a}_2|$ the local unit normal field, $\boldsymbol{D}_\alpha := (\Lambda_{\sigma\alpha}^p - B_{\sigma\alpha})\boldsymbol{a}^\sigma + \Lambda_\alpha^p \boldsymbol{n}$, $\boldsymbol{d} := \Delta_\alpha^p \boldsymbol{a}^\alpha + (\Delta^p + 1)\boldsymbol{n}$, $\boldsymbol{g}_\alpha(\theta^\alpha, \zeta) := \boldsymbol{a}_\alpha(\theta^\alpha) + \zeta \boldsymbol{D}_\alpha(\theta^\alpha)$, and $\boldsymbol{g}_3(\theta^\alpha, \zeta) := \boldsymbol{d}(\theta^\alpha)$. Clearly, $\mathbf{F}^p = \boldsymbol{g}_i \otimes \boldsymbol{G}^i$, as can be seen by comparing $\boldsymbol{g}$ obtained from $(65)_2$ with the expression (43) [59]. The dislocation densities J^i and $\alpha^{\mu k}$ can then be directly read off from their definitions in terms of the torsion $T_{ij}{}^k(\theta^\alpha) := L_{[ij]}^k\big|_{\zeta=0} = \left((F^{p^{-1}})^{kq} F_{q[i,j]}^p\right)\big|_{\zeta=0}$. Therefore, in the absence of disclinations and metric anomalies, the dislocation density fields are expressible in terms of plastic distortion $\mathbb{F}^p$ and other strain fields. An analogous description of the above results can also be given in terms of the elastic distortion field.

5.2 Strain Incompatibility Relations for Sufficiently Thin Kirchhoff–Love Shells with Small Surface Strain Accompanied by Moderate Rotation

We now revisit the strain incompatibility relations (59)–(62), with strain interpreted as the plastic strain, under several simplifying assumptions. First of all, we assume that disclination densities with components $\Theta^{\mu\nu}$, $\Theta^{\mu 3}$, and Θ^μ, and dislocation densities with components $\alpha^{\mu k}$, are identically zero. This is reasonable if we restrict ourselves to sufficiently thin structured surfaces. The allowable anomalies are therefore restricted to the in-surface wedge disclinations Θ^3, the in-surface screw and edge dislocations J^i, and the metric anomalies Q_{kij}. The components $W_{ij}{}^k$ and $W_{ijk} = g_{mk}|_{\zeta=0} W_{ij}{}^m$, appearing on the right-hand-side of (59)–(62), are given by a sum of the contortion and non-metricity tensors, see (36a), as $W_{ij}{}^k = C_{ij}{}^k + M_{ij}{}^k$. For $\alpha^{\mu k} = 0$ and metric given by (45), the components of the contortion tensor, defined in (36b), take a simple form:

$$C_{3\beta}{}^3 = C_{\beta 3}{}^3 = C_{33}{}^i = C_{3\beta 3} = C_{\beta 33} = C_{33i} = 0, \qquad C_{3\beta}{}^\alpha = C_{\beta 3}{}^\alpha = a^{\alpha\nu}\varepsilon_{\nu\beta} J^3, \tag{66a}$$

$$C_{3\beta\alpha} = C_{\beta 3\alpha} = C_{\alpha\beta}{}^3 = C_{\alpha\beta 3} = \varepsilon_{\alpha\beta} J^3, \tag{66b}$$

$$C_{\alpha\beta\mu} = J^\sigma\left(a_{\sigma\beta}\varepsilon_{\mu\alpha} + a_{\sigma\alpha}\varepsilon_{\mu\beta} + a_{\sigma\mu}\varepsilon_{\alpha\beta}\right), \quad \text{and} \quad C_{\alpha\beta}{}^\mu = a^{\mu\nu} C_{\alpha\beta\nu}, \tag{66c}$$

where $\varepsilon_{\alpha\beta} := a^{\frac{1}{2}} e_{\alpha\beta}$. On the other hand, the tensor associated with non-metricity has components

$$M_{33}{}^3 = M_{333} = \frac{1}{2} Q_{333}, \qquad M_{33\alpha} = \frac{1}{2}(2Q_{3\alpha 3} - Q_{\alpha 33}), \qquad M_{33}{}^\alpha = a^{\alpha\beta} M_{33\beta}, \tag{67a}$$

$$M_{3\alpha}{}^3 = M_{\alpha 3}{}^3 = M_{3\alpha 3} = M_{\alpha 33} = \frac{1}{2} Q_{\alpha 33}, \tag{67b}$$

$$M_{3\alpha}{}^\beta = M_{\alpha 3}{}^\beta = \frac{1}{2} a^{\beta\nu}(Q_{3\nu\alpha} - Q_{\nu\alpha 3} + Q_{\alpha 3\nu}), \tag{67c}$$

$$M_{\alpha\beta}{}^3 = M_{\alpha\beta 3} = \frac{1}{2}(Q_{\alpha 3\beta} - Q_{3\beta\alpha} + Q_{\beta\alpha 3}), \tag{67d}$$

$$M_{\alpha\beta\mu} = \frac{1}{2}(Q_{\alpha\mu\beta} - Q_{\mu\beta\alpha} + Q_{\beta\alpha\mu}), \quad \text{and} \quad M_{\alpha\beta}{}^{\mu} = a^{\mu\nu} M_{\alpha\beta\nu}. \tag{67e}$$

We note that, after these forms are substituted into (59)–(62), the in-surface metric anomalies do not appear in (62). In particular, whenever the out-of-surface metric anomalies are absent, the right side of (62) reduces to $a^{\alpha\beta}\varepsilon_{\alpha\rho}\varepsilon_{\beta\sigma}(J^3)^2$ implying that $|\Lambda^p_{[12]}| = a^{\frac{1}{2}}|J^3|$, i.e., the skewness of the plastic bending strain completely characterizes the in-surface screw dislocations. Also, when both disclinations and metric anomalies are altogether absent, (59)–(62) reduces to

$$K_{1212} - \left[b_{11}b_{22} - b_{12}^2\right] = 2\sqrt{a}\, a_{\sigma[1}\partial_{2]}J^{\sigma} - 2C_{[1|\mu 2|}C_{2]1}{}^{\mu} - a\left(J^3\right)^2, \tag{68}$$

$$-\partial_2 b_{11} + \partial_1 b_{12} = \partial_1\left(\sqrt{a}J^3\right) + aJ^2J^3, \tag{69}$$

$$-\partial_2 b_{21} + \partial_1 b_{22} = \partial_2\left(\sqrt{a}J^3\right) + aJ^1J^3, \quad \text{and} \tag{70}$$

$$a^{\alpha\beta}\varepsilon_{\alpha\rho}\varepsilon_{\beta\sigma}a^{-1}\left(\Lambda^p_{[12]}\right)^2 = a^{\alpha\beta}\varepsilon_{\alpha\rho}\varepsilon_{\beta\sigma}\left(J^3\right)^2. \tag{71}$$

These are the local strain incompatibility relations for Kirchhoff–Love shells with in-surface dislocations as the only source of incompatibility.

To further simplify the incompatibility relations, we assume Θ^3 and J^α, upto their first spatial derivatives, to be $O(\epsilon)$, J^3, upto its first spatial derivative, to be $O(\epsilon^{\frac{1}{2}})$, the pure in-surface metric anomalies $Q_{\mu\alpha\beta}$, along with their first spatial derivatives, to be $O(\epsilon)$, and Q_{kij}, with at least one of the indices k, i, or j taking the value 3, along with their first spatial derivatives, to be $O(\epsilon^{\frac{1}{2}})$. These are motivated from the assumed order of in-surface and bending strains. The identical order of the in-surface strain and the in-surface defects (except J^3), and of the bending strain and out-of-surface defects (along with J^3), restricts the magnitude of defect density fields to comply with the respective strains and the resulting deformation. The assumed order of defect densities also has a direct bearing on the physical phenomena for which these equations could be used. For instance, the defect mediated melting of 2-dimensional solid crystals would require defect densities to proliferate beyond an order of magnitude that is otherwise allowed in the present framework [51, Chap. 6].

We will now simplify the incompatibility relations (59)–(62) under the stated assumptions on defect densities and metric anomalies in addition to the restriction of small strain accompanied by moderate rotation, i.e., $E^p_{\alpha\beta} = O(\epsilon)$ and $\Lambda^p_{\alpha\beta} = O(\epsilon^{\frac{1}{2}})$. We begin by noting that $a = A(1 + 2A^{\alpha\mu}E^p_{\alpha\mu}) + o(\epsilon)$, where $A := \det[A_{\alpha\beta}]$, and $a^{\alpha\beta} = A^{\alpha\beta} - 2E^{p\alpha\beta} + o(\epsilon)$, where $E^{p\alpha\beta} := A^{\alpha\rho}A^{\beta\sigma}E^p_{\rho\sigma} = O(\epsilon)$. Consequently, $s^{\tau}_{\alpha\beta} = \bar{s}^{\tau}_{\alpha\beta} + H^p_{\alpha\beta}{}^{\tau} + o(\epsilon)$, where $\bar{s}^{\tau}_{\alpha\beta} := \frac{1}{2}A^{\tau\sigma}(A_{\sigma\beta,\alpha} + A_{\sigma\alpha,\beta} - A_{\alpha\beta,\sigma})$ are the surface Christoffel symbols on the reference configuration and $H^p_{\alpha\beta}{}^{\tau} := A^{\tau\nu}(\bar{\partial}_\alpha E^p_{\nu\beta} + \bar{\partial}_\beta E^p_{\nu\alpha} - \bar{\partial}_\nu E^p_{\alpha\beta}) = O(\epsilon)$; here, recall that, $\bar{\partial}$ denotes the surface covariant derivative on the reference configuration with respect to $\bar{s}$. Moreover, upto $O(\epsilon)$, $K_{\beta\alpha\mu\nu} = \bar{K}_{\beta\alpha\mu\nu} + 2\bar{\partial}_{[\beta}H^p_{\alpha]\mu\nu}$, where $\bar{K}_{\beta\alpha\mu\nu}$ are the components of the Riemann–Christoffel curvature obtained from $\bar{s}$. Also, $b_{11}b_{22} - b_{12}^2 = B_{11}B_{22} - B_{12}^2 + \{\Lambda^p_{11}\Lambda^p_{22} - (\Lambda^p_{(12)})^2\}$ upto $O(\epsilon)$. Using the last two relations, and the fact that the pair $(A_{\alpha\beta}, B_{\alpha\beta})$ satisfies the Gauss and Codazzi–Mainardi equations on the reference configuration, we obtain, upto $O(\epsilon)$,

$$K_{1212} + \left[b_{11}b_{22} - b_{12}^2\right] = \bar{\partial}_{11}E^p_{22} + \bar{\partial}_{22}E^p_{11} - 2\bar{\partial}_2\bar{\partial}_1E^p_{12} + \left\{\Lambda^p_{11}\Lambda^p_{22} - \left(\Lambda^p_{(12)}\right)^2\right\}. \tag{72}$$

Additionally, due to $\partial_\alpha b_{\mu\nu} = -\bar{\partial}_\alpha \Lambda^p_{(\mu\nu)} + \bar{\partial}_\alpha B_{\mu\nu} + O(\epsilon)$, we have, upto $O(\epsilon^{\frac{1}{2}})$,

$$-\partial_2 b_{\mu 1} + \partial_1 b_{\mu 2} = \bar{\partial}_2 \Lambda^p_{(\mu 1)} - \bar{\partial}_1 \Lambda^p_{(\mu 2)}. \tag{73}$$

Substituting (72) and (73) into (59)–(62), and using the order assumptions on the defect densities, we finally obtain

$$\bar{\partial}_{11} E^p_{22} + \bar{\partial}_{22} E^p_{11} - 2\bar{\partial}_2\bar{\partial}_1 E^p_{12} + \Lambda^p_{11}\Lambda^p_{22} - \left(\Lambda^p_{(12)}\right)^2$$
$$= A\Theta^3 + 2\sqrt{A}\, A_{\sigma[1}\bar{\partial}_{2]} J^\sigma - 2\bar{\partial}_{[1} M_{2]12} - 2M_{[1|32|}\, M_{2]1}{}^3, \tag{74}$$

$$\bar{\partial}_2 \Lambda^p_{11} - \bar{\partial}_1 \Lambda^p_{(12)} = \sqrt{A}\bar{\partial}_1 J^3 - 2\bar{\partial}_{[1} M_{2]13} - 2M_{[1|33|}\, M_{2]1}{}^3, \tag{75}$$

$$\bar{\partial}_2 \Lambda^p_{(21)} - \bar{\partial}_1 \Lambda^p_{22} = \sqrt{A}\bar{\partial}_2 J^3 - 2\bar{\partial}_{[1} M_{2]23} - 2M_{[1|33|}\, M_{2]2}{}^3, \quad \text{and} \tag{76}$$

$$A^{-1}A^{\alpha\beta} e_{\alpha\rho} e_{\beta\sigma}\left(\Lambda^p_{[12]}\right)^2 = A^{-1}A^{\alpha\beta} e_{\alpha\rho} e_{\beta\sigma}\left(J^3\right)^2 - M_{\rho\alpha}{}^3 M_{3\sigma}{}^\alpha - M_{\rho 3}{}^3 M^3_{\sigma 3} + M_{33}{}^3 M^3_{\rho\sigma} \tag{77}$$

as the local strain incompatibility conditions for sufficiently thin Kirchhoff–Love shells written in terms of the plastic strain fields. The equations (74) and (77) are $O(\epsilon)$, whereas (75) and (76) are $O(\epsilon^{\frac{1}{2}})$. In Sect. 5.3, we will combine these equations with constitutive assumptions and equilibrium conditions. The incompatibility equations (74)–(77), even in this simplified form, have not appeared elsewhere.

Remark 3 (Strain incompatibility relation for thin flexible plates) To reduce the incompatibility relations (59)–(62) for perfectly flexible plate like structures, e.g., a thin sheet of paper, which allow large bending strain but vanishingly small in-surface stretching, we take the reference surface to be flat, i.e., $B_{\alpha\beta} = 0$, and identify the curvilinear coordinates (θ^1, θ^2) with the Cartesian coordinates, i.e., $A_{\alpha\beta} = \delta_{\alpha\beta}$. The covariant derivatives then get replaced by the ordinary partial derivatives. Also, due to the absence of surface strains, $a_{\alpha\beta} = A_{\alpha\beta} = a^{\alpha\beta} = A^{\alpha\beta} = \delta_{\alpha\beta}$; hence $a = A = 1$, $s^\mu_{\alpha\beta} = 0$, $K = 0$. For the purpose of this remark, we do not assume any order assumption on the defect densities. The local strain incompatibility equations (59)–(62) then reduce to

$$\left(\Lambda^p_{(12)}\right)^2 - \Lambda^p_{11}\Lambda^p_{22} = \Theta^3 - 2\partial_{[1} W_{2]12} - 2W_{[1|i2|}\, W_{2]1}{}^i, \tag{78}$$

$$\Lambda^p_{11,2} - \Lambda^p_{(12),1} = -2W_{[2|13|,1]} - 2W_{[1|i3|}\, W_{2]1}{}^i, \tag{79}$$

$$\Lambda^p_{(12),2} - \Lambda^p_{22,1} = -2W_{[2|23|,1]} - 2W_{[1|i3|}\, W_{2]2}{}^i, \quad \text{and} \tag{80}$$

$$e_{\alpha\rho} e_{\alpha\sigma}\left(\Lambda^p_{[12]}\right)^2 = -M_{3\sigma}{}^3{}_{,\rho} - \left(C_{\rho\alpha}{}^3 + M_{\rho\alpha}{}^3\right)\left(C_{3\sigma}{}^\alpha + M_{3\sigma}{}^\alpha\right)$$
$$- M_{\rho 3}{}^3 M^3_{\sigma 3} + M_{3\alpha}{}^3 W^\alpha_{\rho\sigma} + M_{33}{}^3 W^3_{\rho\sigma}. \tag{81}$$

These provide a complete system of partial differential algebraic equations for the plastic bending strain $\boldsymbol{\Lambda}^p$ with various defect densities as source terms. In the absence of disclinations and metric anomalies, these further reduce down to (compare with (68)–(71))

$$\left(\Lambda^p_{(12)}\right)^2 - \Lambda^p_{11}\Lambda^p_{22} = J^1_{,2} - J^2_{,1} - \left(J^3\right)^2, \tag{82}$$

$$\Lambda^p_{11,2} - \Lambda^p_{(12),1} = J^3_{,1} + J^2 J^3, \tag{83}$$

$$\Lambda^p_{(12),2} - \Lambda^p_{22,1} = J^3_{,2} + J^1 J^3, \quad \text{and} \quad |\Lambda^p_{[12]}| = |J^3|. \tag{84}$$

The above relations have been earlier obtained by Derezin [16], although with erroneous terms. On the other hand, if dislocations and metric anomalies are both absent, the plastic bending strain is symmetric and can always be written as $\Lambda^p_{\alpha\beta} = w^p_{,\alpha\beta}$ for some scalar field w^p defined over simply connected open sets $U \subset \omega$. The plastic Gaussian curvature of the material space $(\Lambda^p_{12})^2 - \Lambda^p_{11}\Lambda^p_{22}$ is then given by the wedge disclination density Θ^3; this is then the only non-trivial incompatibility equation.

5.3 Föppl–von Kármán Equations with Incompatible Elastic Strain for Shells with Arbitrary Reference Geometry

The equilibrium equations in the classical Föppl–von Kármán theory for thin elastic shells are given by the localized in-plane and vertical force balance relations [45]

$$\bar{\partial}_\beta \sigma^{\alpha\beta} = 0 \quad \text{and} \quad \sigma^{\alpha\beta}\Lambda_{\alpha\beta} + \bar{\partial}_{\alpha\beta} M^{\alpha\beta} = 0, \tag{85}$$

where the 2-dimensional linear stress-strain and bending moment-bending strain relations, upto $O(\epsilon)$ and $O(\epsilon^{\frac{1}{2}})$, respectively, are taken as

$$\begin{aligned}\sigma^{\alpha\beta} &= \frac{E}{(1-\nu^2)}\Big(\nu E^e_{\mu\mu} A^{\alpha\beta} + (1-\nu) E^e_{\mu\nu} A^{\mu\alpha} A^{\nu\beta}\Big) \quad \text{and} \\ M^{\alpha\beta} &= D\Big(\nu \Lambda^e_{\mu\mu} A^{\alpha\beta} + (1-\nu)\Lambda^e_{\mu\nu} A^{\mu\alpha} A^{\nu\beta}\Big).\end{aligned} \tag{86}$$

The scalars E, ν, and D are material constants. Equation $(85)_1$ is identically satisfied when the stress components $\sigma^{\alpha\beta}$ are expressed in terms of the 2-dimensional Airy stress function $\Phi(\theta^\alpha)$ over the reference configuration as $\sigma^{\alpha\beta} = \bar{\varepsilon}^{\alpha\mu}\bar{\varepsilon}^{\beta\nu}\bar{\partial}_{\mu\nu}\Phi$, where $\bar{\varepsilon}^{\alpha\mu} = A^{-\frac{1}{2}} e^{\alpha\mu}$. On the other hand, $(85)_2$, after writing stress in terms of the stress function, recalling the decomposition (64b), and using the constitutive relation $(86)_2$, reduces to

$$D\big(\nu A^{\mu\nu} A^{\alpha\beta} + (1-\nu) A^{\mu\alpha} A^{\nu\beta}\big)\, \bar{\partial}_{\alpha\beta} \Lambda_{\mu\nu} + \bar{\varepsilon}^{\alpha\mu}\bar{\varepsilon}^{\beta\nu}\Lambda_{\alpha\beta}\,\bar{\partial}_{\mu\nu}\Phi = D\Omega_p, \tag{87}$$

where $\Omega_p := \big(\nu A^{\mu\nu} A^{\alpha\beta} + (1-\nu) A^{\mu\alpha} A^{\nu\beta}\big)\,\bar{\partial}_{\alpha\beta}\Lambda^p_{(\mu\nu)}$. Additionally, the total strain is compatible and hence satisfies

$$\bar{\partial}_{11} E_{22} + \bar{\partial}_{22} E_{11} - 2\bar{\partial}_{12} E_{12} + \Lambda_{11}\Lambda_{22} - (\Lambda_{12})^2 = 0 \quad \text{and} \tag{88}$$

$$\bar{\partial}_1 \Lambda_{\mu 2} - \bar{\partial}_2 \Lambda_{\mu 1} = 0. \tag{89}$$

We use the additive surface strain decomposition (64a) in (88), and then substitute $E^e_{\alpha\beta} = \frac{1}{E}\big((1+\nu)A_{\alpha\mu}A_{\beta\nu} - \nu A_{\alpha\beta}A_{\mu\nu}\big)\sigma^{\mu\nu}$, obtained using the inverse of the stress-strain relation $(86)_1$, before writing $\sigma^{\mu\nu}$ in terms of the Airy stress function, to obtain

$$\frac{1}{E}\Big[\bar{\partial}_{\alpha\beta}, \big((1+\nu)A_{\alpha\mu}A_{\beta\nu} - \nu A_{\alpha\beta}A_{\mu\nu}\big)\bar{\varepsilon}^{\mu\rho}\bar{\varepsilon}^{\nu\sigma}\,\bar{\partial}_{\rho\sigma}\Phi\Big] + \Lambda_{11}\Lambda_{22} - (\Lambda_{12})^2 = -\lambda_p, \tag{90}$$

where $[C_{\alpha\beta}, D_{\alpha\beta}] := C_{11}D_{22} + C_{22}D_{11} - 2C_{12}D_{12}$ for scalar quantities $C_{\alpha\beta}$ and $D_{\alpha\beta}$, such that $C_{\alpha\beta} = C_{\beta\alpha}$ and $D_{\alpha\beta} = D_{\beta\alpha}$, and $\lambda_p := -2\bar{\partial}_{12}E^p_{12} + \bar{\partial}_{22}E^p_{11} + \bar{\partial}_{11}E^p_{22}$. We call Ω_p the total plastic curvature incompatibility and λ_p the total plastic stretch incompatibility. Equations (87) and (90) constitute the Föppl–von Kármán shell equations with arbitrary reference geometry; they are the governing partial differential equations for the determination of surface stress and out-of-surface deformation, given Ω_p and λ_p. Indeed, consider a global Cartesian reference frame $\mathbf{e}_i$, with the local reference and current configurations of the surface expressed in the Monge forms $\boldsymbol{R}(U) = \theta^\alpha \mathbf{e}_\alpha + \bar{w}(\theta^\alpha)\mathbf{e}_3$ and $\hat{\boldsymbol{R}}(U) = \theta^\alpha \mathbf{e}_\alpha + \hat{w}(\theta^\alpha)\mathbf{e}_3$, respectively; the reference shape $\bar{w}(\theta^\alpha)$ is given. Then $A_{\alpha\beta} = \delta_{\alpha\beta} + \bar{w}_{,\alpha}\bar{w}_{,\beta}$ and $\Lambda_{\alpha\beta} = \bar{w}_{,\alpha\beta}/\sqrt{1+(\bar{w}_{,1})^2+(\bar{w}_{,2})^2} - \hat{w}_{,\alpha\beta}/\sqrt{1+(\hat{w}_{,1})^2+(\hat{w}_{,2})^2}$. The fields Ω_p and λ_p can be expressed in terms of various defect density fields using the strain incompatibility relations, as will be illustrated below.

Remark 4 (Shallow shells) When the reference geometry is moderately curved, the functions $\bar{w}$ and $\hat{w}$, along with their first and second spatial derivatives, are both $O(\epsilon^{\frac{1}{2}})$. As a result, $\Lambda_{\alpha\beta} = (\bar{w} - \hat{w})_{,\alpha\beta}$ upto $O(\epsilon^{\frac{1}{2}})$. Moreover, we can also replace the reference covariant derivatives $\bar{\partial}$ in the above expressions with ordinary partial derivatives while retaining terms upto the leading order. The Föppl–von Kármán equations (87) and (90) then reduce to a form used previously in the context of thermoelasticity and growth [41, 43, 45].

Remark 5 (2-dimensional solid crystals with edge dislocations, wedge disclinations, and in-surface metric anomalies) Assume that the density of screw disclinations and the densities of out-of-surface metric anomalies are identically zero. With this, the local plastic strain incompatibility relations (74)–(77) reduce to

$$\begin{aligned} &\bar{\partial}_{11} E^p_{22} + \bar{\partial}_{22} E^p_{11} - 2\bar{\partial}_2\bar{\partial}_1 E^p_{12} + \Lambda^p_{11}\Lambda^p_{22} - \left(\Lambda^p_{12}\right)^2 \\ &\quad = A\Theta^3 + 2\sqrt{A}\, A_{\sigma[1}\bar{\partial}_{2]} J^\sigma - \bar{\partial}_1 M_{212} + \bar{\partial}_2 M_{112}, \end{aligned} \tag{91}$$

$\bar{\partial}_\alpha \Lambda^p_{\mu\beta} - \bar{\partial}_\beta \Lambda^p_{\mu\alpha} = 0$, and $\Lambda^p_{[\alpha\beta]} = 0$. We can choose $\Lambda^p_{\alpha\beta} \equiv 0$ without any loss of generality. Consequently, $\lambda_p = A\Theta^3 + 2\sqrt{A}\, A_{\sigma[1}\bar{\partial}_{2]} J^\sigma - \bar{\partial}_1 M_{212} + \bar{\partial}_2 M_{112}$ and $\Omega_p \equiv 0$. Our formulation then reduces to that used in the condensed matter literature on curved 2-dimensional crystals [8] [51, Chap. 6]. In the mentioned literature, however, only discrete disclinations and dislocations were considered in the form of dirac distributions, and only isotropic point-defect densities were considered, such that $Q_{\mu\alpha\beta} = \phi_{,\mu} A_{\alpha\beta}$, where the scalar field $\phi(\theta^\alpha)$ provides a measure of the distributed point defects [60].

Remark 6 (Growing biological surfaces) Consider growth of biological surfaces where disclinations and dislocations are both absent. In such a scenario, metric anomalies can be represented in terms of the symmetric quasi-plastic strain fields $\tilde{q}_{ij} : W \times (-\epsilon, \epsilon) \to \mathbb{R}$ as $Q_{kij}(\theta^\alpha) = -2\tilde{q}_{ij;k}\big|_{\zeta=0}$ over simply connected patches $W \subset \omega$ (see Sect. 3.1.4 for details). We assume the following form of $\tilde{q}_{ij}(\theta^\alpha, \zeta)$:

$$\tilde{q}_{\alpha\beta} = q^0_{\alpha\beta} - 2\zeta q'_{\alpha\beta} + \zeta^2 A^{\mu\nu} q'_{\alpha\mu} q'_{\nu\beta},\ \tilde{q}_{\alpha 3} = \tilde{q}_{3\alpha} = 0, \quad \text{and} \quad \tilde{q}_{33} = 1, \tag{92}$$

where the symmetric functions $q^0_{\alpha\beta}(\theta^\alpha)$, along with their first derivatives, and $q'_{\alpha\beta}(\theta^\alpha)$ are $O(\epsilon)$ and $O(\epsilon^{\frac{1}{2}})$, respectively. The above expression is motivated by the form (45) of the material metric for Kirchhoff–Love shells with small in-surface strain accompanied by moderate rotations. We obtain $Q_{\mu\alpha\beta} = -2\bar{\partial}_\mu q^0_{\alpha\beta}$, upto $O(\epsilon)$, $Q_{3\alpha\beta} = 4q'_{\alpha\beta}$, upto $O(\epsilon^{\frac{1}{2}})$, and $Q_{k33} = Q_{k\alpha 3} = Q_{k3\alpha} = 0$. Accordingly, the functions $q^0_{\alpha\beta}$ measure the in-surface metric anomalies, e.g., surface growth, whereas $q'_{\alpha\beta}$ measure the tangential differential surface growth along the thickness direction. The plastic strain incompatibility relations (74)–(77) reduce to

$$\begin{aligned}&\bar{\partial}_{11} E^p_{22} + \bar{\partial}_{22} E^p_{11} - 2\bar{\partial}_2 \bar{\partial}_1 E^p_{12} + \Lambda^p_{11}\Lambda^p_{22} - \left(\Lambda^p_{(12)}\right)^2 \\ &\quad = \bar{\partial}_{11} q^0_{22} + \bar{\partial}_{22} q^0_{11} - 2\bar{\partial}_2\bar{\partial}_1 q^0_{12} + 4\left(q'_{11}q'_{22} - \left(q'_{12}\right)^2\right),\end{aligned} \tag{93}$$

$$\bar{\partial}_2 \Lambda^p_{11} - \bar{\partial}_1 \Lambda^p_{(12)} = 2\left(\bar{\partial}_1 q'_{12} - \bar{\partial}_2 q'_{11}\right), \tag{94}$$

$$\bar{\partial}_2 \Lambda^p_{(21)} - \bar{\partial}_1 \Lambda^p_{22} = 2\left(\bar{\partial}_1 q'_{22} - \bar{\partial}_2 q'_{21}\right), \quad \text{and} \tag{95}$$

$$\left(\Lambda^p_{[12]}\right)^2 = \frac{4AA^{\alpha\beta}q'_{1\alpha}q'_{1\beta}}{A^{22}} = \frac{4AA^{\alpha\beta}q'_{2\alpha}q'_{2\beta}}{A^{11}} = -\frac{4AA^{\alpha\beta}q'_{1\alpha}q'_{2\beta}}{A^{12}}. \tag{96}$$

The relations (96) can be interpreted as restrictions on the functions $q'_{\alpha\beta}$. We readily make the identifications $E^p_{\alpha\beta} = q^0_{\alpha\beta}$ and $\Lambda^p_{(\alpha\beta)} = -2q'_{\alpha\beta}$. The plastic in-surface strain can then be specified directly by the in-surface growth tensor $q^0_{\alpha\beta}$, and the plastic bending strain field by the tangential differential growth tensor $q'_{\alpha\beta}$. The tangential differential growth along the thickness, hence, acts as a source to the incompatible growth curvature field Ω_p. Furthermore, if the reference configuration is flat, we can choose the coordinate system θ^α to be the Cartesian coordinate system. The relations (96) then lead to $(\Lambda^p_{[12]})^2 = 4((q'_{11})^2 + (q'_{12})^2) = 4((q'_{22})^2 + (q'_{12})^2)$ and $q'_{12}(q'_{11} + q'_{22}) = 0$. The former of these imply $q'_{11} = \pm q'_{22}$. According to the latter, when $q'_{11} = -q'_{22} \neq 0$, q'_{12} may assume any non-zero value, e.g., in tangential differential growth along the thickness. For $q'_{11} = q'_{22} \neq 0$, $q'_{12} = 0$, which is the case of isotropic tangential differential growth along the thickness, we have $|\Lambda^p_{[12]}| = 2|q'_{11}| = 2|q'_{22}|$. Finally, if $q'_{11} = q'_{22} = 0$, q'_{12} may assume any non-zero value, representing the anisotropic tangential differential growth of shear type along the thickness, such that $|\Lambda^p_{[12]}| = 2|q'_{12}|$. The growth of biological surfaces has been studied using Föppl–von Kármán equations for shallow shells in the works of Mahadevan and coauthors [41, 43]. However, they have used the incompatibilities Ω_p and λ_p without interpreting the former in terms of growth strains, as is done above. We also note that there can be alternate geometrical descriptions of surface biological growth [61].

Remark 7 (Fluid films with curvature elasticity) We consider thin isotropic incompressible fluid films with curvature elasticity whose free energy per unit area of the natural configuration of the film is assumed to be of the form $W(\boldsymbol{\Lambda}^e) = \frac{k}{4}(\mathrm{tr}\boldsymbol{\Lambda}^e)^2$, where $k > 0$ is the constant bending modulus [2, 66]. Here $\mathrm{tr}\boldsymbol{\Lambda}^e = a^{\mu\nu}\Lambda^e_{\mu\nu} = a^{\mu\nu}(b_{\mu\nu} - \hat{B}_{\mu\nu})$, where, recall that, $b_{\mu\nu}$ and $\hat{B}_{\mu\nu}$ are the second fundamental forms associated with the surface in the natural and the current configuration, respectively. The assumed strain energy density in fact becomes identical to the Helfrich energy [2, 28] if we identify $\frac{1}{2}a^{\mu\nu}b_{\mu\nu}$, the mean curvature of the surface in the natural configuration, as the non-uniform spontaneous curvature. Indeed, retaining terms only upto leading order, and defining $H := \frac{1}{2}A^{\mu\nu}\hat{B}_{\mu\nu}$, $H^p := \frac{1}{2}A^{\mu\nu}b_{\mu\nu}$, we can write $W = k(H - H^p)^2$. We will use our formalism to derive relations for determining the spontaneous curvature from a given distribution of wedge disclinations over the fluid film. The governing equations for shape determination of the fluid film, with zero external loading, are

$$k\bar{\Delta}\left(H - H^p\right) + 2k\left(H - H^p\right)\left(2H^2 - \hat{K}\right) - 2kH\left(H - H^p\right)^2 - 2\mu H = 0 \tag{97}$$

and $\mu_{,\alpha} = 2k(H - H^p)H^p_{,\alpha}$, where $\bar{\Delta}(\cdot) := \bar{\partial}_{\alpha\beta}(\cdot)A^{\alpha\beta}$ is the surface Laplacian, $\hat{K} := \det(\hat{B}_{\mu\nu})$ is the Gaussian curvature of the surface in the current configuration, and μ is a constitutively undetermined Lagrange multiplier corresponding to the deformation constraint of incompressibility [2, 66]. The solution $\hat{H} = H^p$ and $\mu = 0$ is ruled out, even though it corresponds to a global minimum of the total energy, since H^p may not correspond to any realizable surface isometrically embedded in $\mathbb{R}^3$. The strain incompatibility relations, ignoring surface strains and all the defect densities except Θ^3, require $\Lambda^p_{\alpha\beta}$ to be symmetric and satisfy

$$\Lambda^p_{11}\Lambda^p_{22} - \left(\Lambda^p_{12}\right)^2 = A\Theta^3 \quad \text{and} \quad \bar{\partial}_2\Lambda^p_{\mu 1} - \bar{\partial}_1\Lambda^p_{\mu 2} = 0. \tag{98}$$

The latter relation implies existence of a scalar field w^p such that $\Lambda^p_{\alpha\beta} = w^p_{,\alpha\beta}$. When substituted in the former relation, we obtain an inhomogeneous covariant Monge–Ampère equation $[\bar{\partial}_{\alpha\beta}w^p, \bar{\partial}_{\alpha\beta}w^p] = 2A\Theta^3$ to solve for w^p. The spontaneous curvature H^p can be then calculated using $b_{\mu\nu} = B_{\mu\nu} - \Lambda^p_{\mu\nu}$. For moderately curved films, the shape equation reduces to $(k/2)\hat{w}_{,\alpha\alpha\beta\beta} + \mu\hat{w}_{,\alpha\alpha} = (k/2)w^p_{,\alpha\alpha\beta\beta}$, where $\hat{w}$ determines the shape of the film in the current configuration and w^p is now solution to the standard inhomogeneous Monge–Ampère equation $[w^p_{,\alpha\beta}, w^p_{,\alpha\beta}] = 2A\Theta^3$.

6 Conclusion

The central aim of our work is to provide an unambiguous description of geometry and mechanics of local defects, within a non-Euclidean geometric framework, in structured surfaces. Our results are applicable to rapidly growing class of defective 2-dimensional crystalline and liquid crystalline surfaces, growing biological shell structures, and fluid films with non-uniform spontaneous curvature. The differential geometric framework naturally leads us to describe defects as sources of strain incompatibility, which, with suitably described kinematics and material response, is manifested physically as residual stress and deformed shape of the material surface. Therefore, we have a formulation which can be used to describe the macroscopic mechanical response of a wide variety of 2-dimensional structures for a given distribution of defects.

The present work has been primarily concerned with *local* anomalies in materially uniform simple elastic 2-dimensional bodies. Material defects can also appear as *global* anomalies on structured surfaces. The global defect affects the topology of the surface, rendering them, for instance, multiply connected or non-orientable, as is the case with Möbius and toroidal surface crystals, etc. [8, 26, 27]. Consider, as an example, the self assembly of certain copolymers in colloidosomes, where toroidal micelles are energetically more favourable over spherical or cylindrical topologies within a range of certain physical parameters. In order for the phase transformation to occur from the unstable spherical, or cylindrical, to the stable toroidal topology (driven by some internal or external agency), one or more global defects must be introduced in each spherical/cylindrical droplets of the unstable phase to achieve the new topology [29, 54]. We have made some preliminary attempts to extend the present work to include these global topological defects and revisit the issues of strain incompatibility, stress, and natural shape while emphasizing the geometric interplay between local and global anomalies in structured surfaces [57, 58], see also [73, Chap. 5]. As future work, it will be important to extend existing theories of defective surfaces using our model and demonstrate their wider physical applicability. It will also be imminent to find new areas of application, where available models have otherwise failed, and develop rigorous numerical methodologies for simulation of practical problems.

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