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Conservation laws for defect fields in non-contractible domains

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ABSTRACT

We consider singular dislocation and disclination fields within a three-dimensional, possibly non-contractible, connected domain, given in terms of piecewise smooth bulk densities and as concentrations over internal surfaces and curves. We obtain conservation laws for the defect fields which characterize the admissibility of defect configurations in the domain. The conservation laws necessarily include global (non-local) conditions whenever the domain has a boundary consisting of multiple, mutually disjoint, connected components, as is the case with a hollow ball or a hollow torus. We demonstrate the applicability of the global conditions for several defect configurations in a hollow ball.

1. Introduction

A single dislocation in a three-dimensional (3D) elastic solid is characterized by a constant Burgers vector and a curve which cannot terminate inside the body so as to ensure a well-defined distortion field away from the curve [1]; the curve can either form a loop or end at the boundary of the domain. For a continuous distribution of dislocations, characterized by a smooth density $\boldsymbol{\alpha}_B$ over the domain, we analogously require $\operatorname{div} \boldsymbol{\alpha}_B^T = \mathbf{0}$ to ensure the existence of a smooth distortion field $\boldsymbol{\beta}$ such that $\boldsymbol{\alpha}_B = \operatorname{curl} \boldsymbol{\beta}$ [1]. These restrictions, on an isolated defect curve and on the smooth density field, are however insufficient (for the existence of the distortion field) when the domain is non-contractible with a boundary which consists of multiple, mutually disjoint, connected components. Within a hollow ball, for instance, a regular dislocation curve cannot intersect both the outer and the inner boundary (of the ball) unless there is at least one more dislocation which also intersects both boundaries (see Figs. 1(a) and 1(b)). An admissible dislocation density field over a hollow ball, on the other hand, should be divergence free and should also have a vanishing net flux across the inner boundary (or equivalently across the outer boundary), see Eqs. (21). In this paper we establish such results, which are novel to the best of our knowledge, in a broader framework which allows for continuous as well as singular descriptions of dislocation and disclination fields.

We consider defect fields as distributions given in terms of piecewise smooth densities over a 3D domain, smooth concentrations over internal surfaces, and smooth concentrations over internal curves within the domain [2,3]. Examples of the latter two include defect walls and defect curves. Motivated by the classical defect theory [4], we postulate a relationship between defects and kinematical fields (strain and bend-twist) and ask for the necessary and sufficient conditions on the defect densities for the existence of strain and bend-twist fields which satisfy the posited relationship. The equation connecting dislocation density to the distortion field, as mentioned in the preceding paragraph, is a special case of such a postulation. The necessary and sufficient conditions, given in Eqs. (10) and (11), are derived as a consequence of a theorem by De Rham [5], see Section 3. Due to their mathematical structure and physical significance, these conditions are called conservation laws for the considered defect density fields. Some of the derived conditions are global in the sense that they depend on the overall shape of the domain and are non-trivial only when the 3D domain is non-contractible with a boundary which consists of multiple, mutually disjoint, connected components.

As an immediate application of our results we consider several defect configurations over a hollow ball and emphasize the restrictions imposed by the global conditions, see Section 4. This was already discussed in the context of dislocations above. In the following, we briefly summarize certain implications for disclination curves. In order to satisfy the local conservation laws, isolated disclination curves (without any dislocation content) are necessarily straight lines of a pure wedge character [6]. An isolated disclination line cannot intersect both the boundaries of the ball unless there is at least one more disclination line which does the same. If only two of such disclination lines are present then they should have identical Frank vector and be collinear (see Fig. 1(d)). The pair of disclinations can be non-collinear in the presence of a dislocation curve or a dislocation wall (see Figs. 1(f) and 1(h)). If three disclination lines are present then they necessarily need to be coplanar and meet at a point (see Fig. 1(e)). A non-straight

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disclination can appear if the curve is allowed to have non-trivial dislocation content or if the curve forms an edge of a dislocation wall (see Fig. 1(g)), among other possibilities. Such restrictions have been overlooked in the literature, particularly in the recent works on defective spherical shells [7–9]. We note that our global conditions are distinct from those imposing a net disclination charge on two-dimensional spherical crystals [10], which arise (as a consequence of the Gauss–Bonnet theorem) due to the inherent lattice microstructure of the crystalline domain. In the context of our work, these can be imposed a posteriori in addition to the derived global conditions.

2. Mathematical preliminaries

2.1. Notation

Let $\Omega \subset \mathbb{R}^3$ be a bounded, connected, open set, with a smooth boundary $\partial\Omega$. The boundary $\partial\Omega$ has k mutually disjoint, smooth, connected components given by $\partial\Omega_i$, $0 \leq i \leq k-1$, i.e., $\cup_{0\leq i\leq k-1}\partial\Omega_i = \partial\Omega$ and $\partial\Omega_i \cap \partial\Omega_j = \emptyset$, for any $i \neq j$, where $\emptyset$ is the empty set. We distinguish between two cases: either $k = 1$ or $k > 1$, regardless of whether Ω is simply or multiply connected. In the former case, $\partial\Omega$ has only one connected component (e.g., solid ball, hollow cylinder), and in the latter, $\partial\Omega$ has multiple components which are disjoint with respect to each other (e.g., hollow ball, hollow torus). Let $S \subset \Omega$ be a regular, oriented, surface, with bounded area, having unit normal $\boldsymbol{n}$ and boundary ∂S. If $\partial S - \partial\Omega = \emptyset$, where $A - B$ denotes the difference between sets A and B, then S is either a closed surface or its boundary is completely contained within the boundary of Ω. On the other hand, if $\partial S - \partial\Omega \neq \emptyset$ then at least some part of ∂S lies in the interior of Ω. Let $L \subset \Omega$ be a regular, oriented, smooth curve, with bounded length, having unit tangent $\boldsymbol{t}$ and boundary ∂L. If $\partial L - \partial\Omega = \emptyset$ then L is either a closed curve or its two ends are completely contained within the boundary of Ω. On the other hand, if $\partial L - \partial\Omega \neq \emptyset$ then at least one end of the curve L lies in the interior of Ω. We use dv, da, and dl to represent volume, area, and length measures on Ω, S, and L, respectively.

Let $\mathcal{V}$ be the translational space of $\mathbb{R}^3$ (set of vectors). Let $\{\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3\}$ be a fixed orthonormal right-handed basis in $\mathcal{V}$. The inner product and the cross product of any two vectors $\boldsymbol{u}, \boldsymbol{v} \in \mathcal{V}$ are given by $\langle \boldsymbol{u}, \boldsymbol{v}\rangle \in \mathbb{R}$ and $\boldsymbol{u} \times \boldsymbol{v} \in \mathcal{V}$, respectively. Let Lin be the space of linear transformations from $\mathcal{V}$ to $\mathcal{V}$ (second order tensors). The space of symmetric and skew symmetric second order tensors are denoted by Sym and Skw, respectively. The identity tensor in Lin is denoted by $\boldsymbol{I}$. For $\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w} \in \mathcal{V}$, the dyadic product $\boldsymbol{u} \otimes \boldsymbol{v} \in \mathrm{Lin}$ is defined such that $(\boldsymbol{u} \otimes \boldsymbol{v})\boldsymbol{w} = \langle \boldsymbol{v}, \boldsymbol{w}\rangle \boldsymbol{u}$. For $\boldsymbol{a} \in \mathrm{Lin}$, $\boldsymbol{a}^T$, $\mathrm{sym}(\boldsymbol{a})$, and $\mathrm{skw}(\boldsymbol{a})$ represent the transpose, the symmetric part, and the skew part of $\boldsymbol{a}$, respectively. The axial vector of $\boldsymbol{b} \in \mathrm{Skw}$ is $ax(\boldsymbol{b}) \in \mathcal{V}$ such that, for any $\boldsymbol{v} \in \mathcal{V}$, $\boldsymbol{b}\boldsymbol{v} = ax(\boldsymbol{b}) \times \boldsymbol{v}$. For $\boldsymbol{a}, \boldsymbol{c} \in \mathrm{Lin}$, the inner product is given by $\langle \boldsymbol{a}, \boldsymbol{c}\rangle \in \mathbb{R}$. The trace of $\boldsymbol{a} \in \mathrm{Lin}$ is defined as $\mathrm{tr}(\boldsymbol{a}) = \langle \boldsymbol{a}, \boldsymbol{I}\rangle$. The cross product of a vector $\boldsymbol{v} \in \mathcal{V}$ with a tensor $\boldsymbol{a} \in \mathrm{Lin}$ is a tensor $(\boldsymbol{v} \times \boldsymbol{a}) \in \mathrm{Lin}$ such that $(\boldsymbol{v} \times \boldsymbol{a})\boldsymbol{u} = (\boldsymbol{v} \times \boldsymbol{a}\boldsymbol{u})$, for all $\boldsymbol{u} \in \mathcal{V}$. We use $C^\infty(\Omega)$, $C^\infty(\Omega, \mathcal{V})$, and $C^\infty(\Omega, \mathrm{Lin})$ to represent spaces of smooth scalar valued, vector valued, and tensor valued functions on Ω, respectively. For a function f on Ω and a subset $\omega \subset \Omega$, $f|_\omega$ is the restriction of f to the subset ω.

We denote the gradient, the divergence, and the curl of a smooth function on Ω with ∇, div, and curl, respectively. Analogously, the surface gradient, the surface divergence, and the surface curl of a smooth function on S are denoted by ∇_S, div_S, and curl_S, respectively [3]. In particular, the surface curl of $\boldsymbol{v} \in C^\infty(S, \mathcal{V})$ is a smooth vector field $\mathrm{curl}_S\, \boldsymbol{v} \in C^\infty(S, \mathcal{V})$ defined as $\langle \mathrm{curl}_S\, \boldsymbol{v}, \boldsymbol{d}\rangle = \mathrm{div}_S(\boldsymbol{v} \times \boldsymbol{d})$, for a fixed $\boldsymbol{d} \in \mathcal{V}$.

2.2. Distributions and their derivatives

Let the spaces of compactly supported smooth functions from Ω to $\mathbb{R}$, $\mathcal{V}$, and Lin be $\mathcal{D}(\Omega)$, $\mathcal{D}(\Omega, \mathcal{V})$, and $\mathcal{D}(\Omega, \mathrm{Lin})$, respectively. The spaces of scalar, vector, and tensor valued distributions, represented as $\mathcal{D}'(\Omega)$, $\mathcal{D}'(\Omega, \mathcal{V})$, and $\mathcal{D}'(\Omega, \mathrm{Lin})$, respectively, are the spaces of all linear continuous functions on $\mathcal{D}(\Omega)$, $\mathcal{D}(\Omega, \mathcal{V})$, and $\mathcal{D}(\Omega, \mathrm{Lin})$, respectively [3, 11]. The product of a scalar function $f \in C^\infty(\Omega)$ with a distribution $T \in \mathcal{D}'(\Omega)$ is a distribution $fT \in \mathcal{D}'(\Omega)$ such that $(fT)(\phi) = T(f\phi)$ for all $\phi \in \mathcal{D}(\Omega)$. The gradient of a scalar distribution $T \in \mathcal{D}'(\Omega)$ is a vector valued distribution $\nabla T \in \mathcal{D}'(\Omega, \mathcal{V})$ such that $\nabla T(\boldsymbol{\phi}) = -T(\mathrm{div}\, \boldsymbol{\phi})$, for all $\boldsymbol{\phi} \in \mathcal{D}(\Omega, \mathcal{V})$. The gradient of a vector valued distribution $\boldsymbol{T} \in \mathcal{D}'(\Omega, \mathcal{V})$ is a tensor valued distribution $\nabla \boldsymbol{T} \in \mathcal{D}'(\Omega, \mathrm{Lin})$ such that $\nabla \boldsymbol{T}(\boldsymbol{\phi}) = -\boldsymbol{T}(\mathrm{div}\, \boldsymbol{\phi})$, for all $\boldsymbol{\phi} \in \mathcal{D}(\Omega, \mathrm{Lin})$. The divergence of a vector valued distribution $\boldsymbol{T} \in \mathcal{D}'(\Omega, \mathcal{V})$ is a scalar valued distribution $\mathrm{Div}\, \boldsymbol{T} \in \mathcal{D}'(\Omega)$ such that $\mathrm{Div}\, \boldsymbol{T}(\phi) = -\boldsymbol{T}(\nabla\phi)$, for all $\phi \in \mathcal{D}(\Omega)$. The divergence of a tensor valued distribution $\boldsymbol{T} \in \mathcal{D}'(\Omega, \mathrm{Lin})$ is a vector valued distribution $\mathrm{Div}\, \boldsymbol{T} \in \mathcal{D}'(\Omega, \mathcal{V})$ such that $\mathrm{Div}\, \boldsymbol{T}(\boldsymbol{\phi}) = -\boldsymbol{T}(\nabla\boldsymbol{\phi})$, for all $\boldsymbol{\phi} \in \mathcal{D}(\Omega, \mathcal{V})$. The curl of a vector valued distribution $\boldsymbol{T} \in \mathcal{D}'(\Omega, \mathcal{V})$ is a vector valued distribution $\mathrm{Curl}\, \boldsymbol{T} \in \mathcal{D}'(\Omega, \mathcal{V})$ such that $(\mathrm{Curl}\, \boldsymbol{T})(\boldsymbol{\phi}) = \boldsymbol{T}(\mathrm{curl}\, \boldsymbol{\phi})$, for all $\boldsymbol{\phi} \in \mathcal{D}(\Omega, \mathcal{V})$. The curl of a tensor valued distribution $\boldsymbol{T} \in \mathcal{D}'(\Omega, \mathrm{Lin})$ is a tensor valued distribution $\mathrm{Curl}\, \boldsymbol{T} \in \mathcal{D}'(\Omega, \mathrm{Lin})$ such that $(\mathrm{Curl}\, \boldsymbol{T})(\boldsymbol{\phi}^T) = \boldsymbol{T}\left((\mathrm{curl}\, \boldsymbol{\phi})^T\right)$, for all $\boldsymbol{\phi} \in \mathcal{D}(\Omega, \mathrm{Lin})$.

2.3. A consequence of De Rham's theorem

For a smooth vector valued function $\boldsymbol{v} \in C^\infty(\Omega, \mathcal{V})$, over a domain Ω whose boundary has only one disjoint component ($k = 1$), the necessary and sufficient condition for there to exist a $\boldsymbol{u} \in C^\infty(\Omega, \mathcal{V})$ such that $\mathrm{curl}\, \boldsymbol{u} = \boldsymbol{v}$ is given by $\mathrm{div}\, \boldsymbol{v} = 0$. For our purposes, however, we need a generalization of this result for distributions over domains whose boundary have multiple, mutually disjoint, components ($k > 1$). We obtain the required result, stated in the following lemma, using De Rham's theorem [5, Theorem 17'] which gives the necessary and sufficient conditions for an arbitrary current to be exact on an arbitrary manifold. The lemma is derived from De Rham's theorem in the supplementary document.

Lemma 2.1. *Given a distribution $\boldsymbol{P} \in \mathcal{D}'(\Omega, \mathcal{V})$ there exists $\boldsymbol{Q} \in \mathcal{D}'(\Omega, \mathcal{V})$ such that $\mathrm{Curl}\, \boldsymbol{Q} = \boldsymbol{P}$ if and only if $\boldsymbol{P}(\boldsymbol{\phi}) = 0$ for all $\boldsymbol{\phi} \in \mathcal{D}(\Omega, \mathcal{V})$ such that $\mathrm{curl}\, \boldsymbol{\phi} = \boldsymbol{0}$.*

In the next lemma, we obtain a useful characterization of the curl free compactly supported smooth vector valued functions, i.e., for $\boldsymbol{\phi} \in \mathcal{D}(\Omega, \mathcal{V})$ such that $\mathrm{curl}\, \boldsymbol{\phi} = \boldsymbol{0}$.

Lemma 2.2. *Given a compactly supported vector valued function $\boldsymbol{\phi} \in \mathcal{D}(\Omega, \mathcal{V})$ such that $\mathrm{curl}\, \boldsymbol{\phi} = \boldsymbol{0}$, there exists a smooth function $u \in C^\infty(\Omega)$ which satisfies $\nabla u = \boldsymbol{\phi}$ in Ω and $u = c_i$ on $\partial\Omega_i$, where $c_i \in \mathbb{R}$ are constants with $c_0 = 0$.*

Proof. Since $\boldsymbol{\phi}$ is compactly supported, $\int_{L_0} \langle \boldsymbol{\phi}, \boldsymbol{t}\rangle\, \mathrm{dl} = 0$ for any loop $L_0 \subset \partial\Omega$. Given $\mathrm{curl}\, \boldsymbol{\phi} = \boldsymbol{0}$, we can therefore write $\int_L \langle \boldsymbol{\phi}, \boldsymbol{t}\rangle\, \mathrm{dl} = 0$ for any loop $L \subset \Omega$, regardless of whether Ω is simply connected or not. Consequently, there exists a $u \in C^\infty(\Omega)$ such that $\nabla u = \boldsymbol{\phi}$ in Ω. Moreover, $\nabla u = 0$ on $\partial\Omega_i$ due to $\boldsymbol{\phi}$ being compactly supported in Ω. Therefore u is constant on $\partial\Omega_i$, i.e., $u = c_i$ on $\partial\Omega_i$ where $c_i \in \mathbb{R}$ are constants, out of which one constant, say c_0, can be taken as 0, without any loss of generality. □

2.4. Identities

We consider $\boldsymbol{B} \in \mathcal{D}'(\Omega, \mathrm{Lin})$, $\boldsymbol{C} \in \mathcal{D}'(\Omega, \mathrm{Lin})$, and $\boldsymbol{H} \in \mathcal{D}'(\Omega, \mathrm{Lin})$ of the form $\boldsymbol{B}(\boldsymbol{\psi}) = \int_\Omega \langle \boldsymbol{b}, \boldsymbol{\psi}\rangle\, \mathrm{dv}$, $\boldsymbol{C}(\boldsymbol{\psi}) = \int_S \langle \boldsymbol{c}, \boldsymbol{\psi}\rangle\, \mathrm{da}$, and $\boldsymbol{H}(\boldsymbol{\psi}) = \int_L \langle \boldsymbol{h}, \boldsymbol{\psi}\rangle\, \mathrm{dl}$, for $\boldsymbol{\psi} \in \mathcal{D}(\Omega, \mathrm{Lin})$, where $\boldsymbol{b} \in \mathrm{Lin}$ is a piecewise smooth bounded function on Ω, possibly discontinuous across S, $\boldsymbol{c} \in \mathrm{Lin}$ is a smooth bounded function on S, and $\boldsymbol{h} \in \mathrm{Lin}$ is a smooth bounded function on L. The discontinuity in $\boldsymbol{b}$ is assumed to be a smooth function on S. If $\partial S - \partial \Omega \neq \emptyset$ then it should vanish as one approaches the boundaries of S within Ω. For $x \in S$, $[\![\boldsymbol{b}]\!](x) = \boldsymbol{b}^+(x) - \boldsymbol{b}^-(x)$, where $\boldsymbol{b}^{\pm}(x)$ are the limiting values of $\boldsymbol{b}$ at x on S from Ω (the − value is from the side into which $\boldsymbol{n}$ points), represents the discontinuity in $\boldsymbol{b}$. The following identities, whose proof is straightforward [3], will be useful for our later calculations.

Identities 2.1. Let $\boldsymbol{u} \in C^\infty(\Omega, \mathcal{V})$ be a vector valued smooth function which satisfies $\boldsymbol{u} = \boldsymbol{c}_i$ on $\partial\Omega_i$, where $\boldsymbol{c}_i \in \mathcal{V}$ are vector valued constants with $\boldsymbol{c}_0 = \boldsymbol{0}$, and whose gradient is a tensor valued compactly supported smooth function, i.e. $\nabla \boldsymbol{u} \in \mathcal{D}(\Omega, \mathrm{Lin})$. Then,

$$\boldsymbol{B}(\nabla \boldsymbol{u}) = -\int_\Omega \langle \operatorname{div} \boldsymbol{b}, \boldsymbol{u}\rangle \,\mathrm{dv} + \int_S \langle [\![\boldsymbol{b}]\!]\boldsymbol{n}, \boldsymbol{u}\rangle \,\mathrm{da} + \sum_{1\le i<k-1} \left\langle \boldsymbol{c}_i, \int_{\partial\Omega_i} \boldsymbol{b}\boldsymbol{n}\,\mathrm{da}\right\rangle, \tag{1}$$

$$\boldsymbol{C}(\nabla \boldsymbol{u}) = -\int_S \left\langle \left(\operatorname{div}_S \boldsymbol{c} + \kappa \boldsymbol{c}\boldsymbol{n}\right), \boldsymbol{u}\right\rangle \mathrm{da} + \int_S \left\langle \boldsymbol{c}\boldsymbol{n}, \frac{\partial \boldsymbol{u}}{\partial n}\right\rangle \mathrm{da} + \int_{\partial S - \partial\Omega} \langle \boldsymbol{c}\boldsymbol{\nu}, \boldsymbol{u}\rangle \,\mathrm{dl} + \sum_{1\le i\le k-1} \left\langle \boldsymbol{c}_i, \int_{\partial S\cap\partial\Omega_i} \boldsymbol{c}\boldsymbol{\nu}\,\mathrm{dl}\right\rangle, \tag{2}$$

where $\partial \boldsymbol{u}/\partial n = (\nabla \boldsymbol{u})\boldsymbol{n}$ is the derivative along $\boldsymbol{n}$, κ is twice the mean curvature of surface S, and $\boldsymbol{\nu} = \boldsymbol{n} \times \boldsymbol{t}$ is the in-plane outward normal to the edge of the surface S, and

$$\boldsymbol{H}(\nabla \boldsymbol{u}) = \int_L \langle \boldsymbol{h}(\boldsymbol{I} - \boldsymbol{t}\otimes\boldsymbol{t}), \nabla \boldsymbol{u}\rangle \,\mathrm{dl} - \int_L \left\langle \frac{\partial(\boldsymbol{h}\boldsymbol{t})}{\partial t}, \boldsymbol{u}\right\rangle \mathrm{dl} + (\langle \boldsymbol{h}\boldsymbol{t}, \boldsymbol{u}\rangle)|_{\partial L - \partial\Omega} + \sum_{1\le i\le k-1} \left\langle \boldsymbol{c}_i, (\boldsymbol{h}\boldsymbol{t})|_{\partial L\cap\partial\Omega_i}\right\rangle, \tag{3}$$

where $\partial(\cdot)/\partial t$ is the tangential derivative along $\boldsymbol{t}$. The restriction $(\cdot)|_{\partial L}$ evaluates the value of $(\cdot)$ at the boundary of L taking into consideration the orientation of L at the end point ∂L.

3. Defect densities and conservation laws

In the classical micromechanical theory of defects in linear elastic solids [4], smooth bulk densities of dislocations and disclinations (denoted by $\boldsymbol{\alpha}_B \in C^\infty(\Omega, \mathrm{Lin})$ and $\boldsymbol{\theta}_B \in C^\infty(\Omega, \mathrm{Lin})$, respectively) are related to smooth strain and bend-twist fields (denoted by $\boldsymbol{\epsilon} \in C^\infty(\Omega, \mathrm{Sym})$ and $\boldsymbol{\kappa} \in C^\infty(\Omega, \mathrm{Lin})$, respectively) as $\boldsymbol{\theta}_B = \operatorname{curl} \boldsymbol{\kappa}^T$ and $\boldsymbol{\alpha}_B = \operatorname{curl} \boldsymbol{\epsilon} + \operatorname{tr}(\boldsymbol{\kappa})\boldsymbol{I} - \boldsymbol{\kappa}^T$. The necessary and sufficient conditions on $\boldsymbol{\theta}_B$ and $\boldsymbol{\alpha}_B$ for there to exist $\boldsymbol{\epsilon}$ and $\boldsymbol{\kappa}$ fields, such that these equations are satisfied for a domain with a single connected boundary component ($k = 1$), are $\operatorname{div} \boldsymbol{\theta}_B^T = \boldsymbol{0}$ and $\operatorname{div} \boldsymbol{\alpha}_B^T + ax(\boldsymbol{\theta}_B^T - \boldsymbol{\theta}_B) = \boldsymbol{0}$. For a vanishing disclination density, i.e., $\boldsymbol{\theta}_B = \boldsymbol{0}$, there exist an infinitesimal rotation field $\boldsymbol{\omega} \in C^\infty(\Omega, \mathrm{Skw})$ such that $\boldsymbol{\kappa}^T = \nabla ax(\boldsymbol{\omega})$ and a distortion field $\boldsymbol{\beta} \in C^\infty(\Omega, \mathrm{Lin})$ such that $\boldsymbol{\beta} = \boldsymbol{\epsilon} + \boldsymbol{\omega}$ and $\boldsymbol{\alpha}_B = \operatorname{curl} \boldsymbol{\beta}$. The integrability condition on $\boldsymbol{\alpha}_B$ is then given by $\operatorname{div} \boldsymbol{\alpha}_B^T = \boldsymbol{0}$. The necessary and sufficient conditions on $\boldsymbol{\theta}_B$ and $\boldsymbol{\alpha}_B$, as discussed above, are called conservation laws for the defect densities; they provide restrictions on the defect distribution such that the defect densities remain consistent with the underlying kinematics of the solid continua. A prescription of defect densities over the body cannot be therefore arbitrary and should necessarily conform to these conditions [4]. The defect conservation laws are closely related to the Bianchi Padova identities in classical differential geometry [12,13]. Our interest is to obtain the conservation laws when the defect densities are additionally allowed to concentrate on surfaces and curves (as in a dislocation/disclination wall or a dislocation/disclination loop) and when the domain Ω has a boundary which has multiple mutually disjoint components ($k > 1$).

We introduce distributional forms of the defect and kinematic fields with $\boldsymbol{K} \in \mathcal{D}'(\Omega, \mathrm{Lin})$ representing the distributional bend-twist field, $\boldsymbol{E} \in \mathcal{D}'(\Omega, \mathrm{Sym})$ the distributional strain field, $\boldsymbol{\Theta} \in \mathcal{D}'(\Omega, \mathrm{Lin})$ the distributional disclination density field, and $\boldsymbol{A} \in \mathcal{D}'(\Omega, \mathrm{Lin})$ the distributional dislocation density field, all defined for a non-contractible domain $\Omega \subset \mathbb{R}^3$ as introduced in Section 2.1. Following the classical relationships between these fields (as mentioned above), we postulate the following equations [3]:

$$\boldsymbol{\Theta} = \operatorname{Curl} \boldsymbol{K}^T \text{ and } \boldsymbol{A} = \operatorname{Curl} \boldsymbol{E} + \operatorname{tr}(\boldsymbol{K})\boldsymbol{I} - \boldsymbol{K}^T. \tag{4}$$

We seek the necessary and sufficient conditions on $\boldsymbol{\Theta}$ and $\boldsymbol{A}$ which would ensure the existence of a bend-twist field $\boldsymbol{K}$ and a strain field $\boldsymbol{E}$ such that they satisfy (4). This problem statement is stated in an alternate but equivalent form in the lemma below.

Lemma 3.1. *For a given distribution of defect densities $\boldsymbol{\Theta} \in \mathcal{D}'(\Omega, \mathrm{Lin})$ and $\boldsymbol{A} \in \mathcal{D}'(\Omega, \mathrm{Lin})$, the existence of distributions $\boldsymbol{K} \in \mathcal{D}'(\Omega, \mathrm{Lin})$ and $\boldsymbol{E} \in \mathcal{D}'(\Omega, \mathrm{Sym})$, satisfying (4), is equivalent to the existence of distributions $\boldsymbol{K} \in \mathcal{D}'(\Omega, \mathrm{Lin})$ and $\boldsymbol{F} \in \mathcal{D}'(\Omega, \mathrm{Lin})$ satisfying $(4)_1$ and*

$$\boldsymbol{A} + (\boldsymbol{x} \times \boldsymbol{\Theta}^T)^T = \operatorname{Curl} \boldsymbol{F}, \tag{5}$$

where $\boldsymbol{x} \in \Omega$ denotes the position vector of a point in Ω.

Proof. Assume that there exist $\boldsymbol{K} \in \mathcal{D}'(\Omega, \mathrm{Lin})$ and $\boldsymbol{E} \in \mathcal{D}'(\Omega, \mathrm{Sym})$ which satisfy (4). Noting the identity

$$\operatorname{Curl}(\boldsymbol{x} \times \boldsymbol{K}^T) = (\boldsymbol{x} \times \boldsymbol{\Theta}^T)^T + \operatorname{tr}(\boldsymbol{K})\boldsymbol{I} - \boldsymbol{K}^T, \tag{6}$$

which follows from $(4)_1$, we can rewrite $(4)_2$ as $\boldsymbol{A} + (\boldsymbol{x} \times \boldsymbol{\Theta}^T)^T = \operatorname{Curl}(\boldsymbol{E} + \boldsymbol{x} \times \boldsymbol{K}^T)$. The desired distribution $\boldsymbol{F} \in \mathcal{D}'(\Omega, \mathrm{Lin})$, defined as $\boldsymbol{F} = \boldsymbol{E} + \boldsymbol{x} \times \boldsymbol{K}^T$, satisfies (5). To prove the converse, assume that there exist distributions $\boldsymbol{K}_1 \in \mathcal{D}'(\Omega, \mathrm{Lin})$ and $\boldsymbol{F} \in \mathcal{D}'(\Omega, \mathrm{Lin})$ which satisfy $\boldsymbol{\Theta} = \operatorname{Curl} \boldsymbol{K}_1^T$ and (5). Using the identity (6) (in terms of $\boldsymbol{K}_1$), we can rewrite (5) as $\boldsymbol{A} = \operatorname{Curl} \boldsymbol{F}_1 + \operatorname{tr}(\boldsymbol{K}_1)\boldsymbol{I} - \boldsymbol{K}_1^T$, where $\boldsymbol{F}_1 = \boldsymbol{F} - (\boldsymbol{x} \times \boldsymbol{K}_1^T)$. The desired distributions $\boldsymbol{K} \in \mathcal{D}'(\Omega, \mathrm{Lin})$ and $\boldsymbol{E} \in \mathcal{D}'(\Omega, \mathrm{Sym})$, defined as $\boldsymbol{K} = \boldsymbol{K}_1 + (\nabla ax(\boldsymbol{S}))^T$ and $\boldsymbol{E} = \operatorname{sym}(\boldsymbol{F}_1)$, where $\boldsymbol{S} = \operatorname{skw}(\boldsymbol{F}_1)$, satisfy (4). The identity $\operatorname{tr}(\nabla ax(\boldsymbol{S}))\boldsymbol{I} - \nabla ax(\boldsymbol{S}) = \operatorname{Curl} \boldsymbol{S}$ is used in proving the preceding assertion. □

The required conditions on $\boldsymbol{\Theta}$ and $\boldsymbol{A}$, as given in the following lemma, follow immediately on using Lemma 2.1 with Lemma 3.1.

Lemma 3.2. *Given $\boldsymbol{\Theta} \in \mathcal{D}'(\Omega, \mathrm{Lin})$ and $\boldsymbol{A} \in \mathcal{D}'(\Omega, \mathrm{Lin})$ there exist distributions $\boldsymbol{K} \in \mathcal{D}'(\Omega, \mathrm{Lin})$ and $\boldsymbol{E} \in \mathcal{D}'(\Omega, \mathrm{Sym})$ such that Eqs. (4) are satisfied if and only if*

$$\boldsymbol{\Theta}(\boldsymbol{\phi}) = 0 \text{ and } \left(\boldsymbol{A} + (\boldsymbol{x} \times \boldsymbol{\Theta}^T)^T\right)(\boldsymbol{\phi}) = 0, \tag{7}$$

for all $\boldsymbol{\phi} \in \mathcal{D}(\Omega, \mathrm{Lin})$ such that $\operatorname{curl} \boldsymbol{\phi} = \boldsymbol{0}$.

In the rest of this section we will derive the consequences of (7) for specific forms of the distributional defect densities. We consider a distributional dislocation density $\boldsymbol{A} \in \mathcal{D}'(\Omega, \mathrm{Lin})$ of the form

$$\boldsymbol{A}(\boldsymbol{\phi}) = \int_\Omega \langle \boldsymbol{\alpha}_B, \boldsymbol{\phi}\rangle \,\mathrm{dv} + \int_S \langle \boldsymbol{\alpha}_S, \boldsymbol{\phi}\rangle \,\mathrm{da} + \int_L \langle \boldsymbol{\alpha}_L, \boldsymbol{\phi}\rangle \,\mathrm{dl}, \tag{8}$$

for $\boldsymbol{\phi} \in \mathcal{D}(\Omega, \mathrm{Lin})$, where $\boldsymbol{\alpha}_B$ is the piecewise smooth bulk dislocation density tensor field over $\Omega - S$, possibly discontinuous across S, $\boldsymbol{\alpha}_S$ is the smooth surface dislocation density tensor field over S, and $\boldsymbol{\alpha}_L$ is the smooth curve dislocation density tensor field over L. Similarly, we consider a distributional disclination density $\boldsymbol{\Theta} \in \mathcal{D}'(\Omega, \mathrm{Lin})$ of the form

$$\boldsymbol{\Theta}(\boldsymbol{\phi}) = \int_\Omega \langle \boldsymbol{\theta}_B, \boldsymbol{\phi}\rangle \,\mathrm{dv} + \int_S \langle \boldsymbol{\theta}_S, \boldsymbol{\phi}\rangle \,\mathrm{da} + \int_L \langle \boldsymbol{\theta}_L, \boldsymbol{\phi}\rangle \,\mathrm{dl}, \tag{9}$$

for $\boldsymbol{\phi} \in \mathcal{D}(\Omega, \mathrm{Lin})$, where $\boldsymbol{\theta}_B$ is the piecewise smooth bulk disclination density tensor field over $\Omega - S$, possibly discontinuous across S, $\boldsymbol{\theta}_S$ is the smooth surface disclination density tensor field over S, and $\boldsymbol{\theta}_L$ is the smooth curve disclination density tensor field over L. Whereas $\boldsymbol{\alpha}_S$ and $\boldsymbol{\theta}_S$ describe defect concentrations over a surface in the domain, as in dislocation/disclination walls and grain boundaries, $\boldsymbol{\alpha}_L$ and $\boldsymbol{\theta}_L$ describe defect concentrations over a curve, as in dislocation/disclination loops. Conditions (7), with $\boldsymbol{A}$ and $\boldsymbol{\Theta}$ given as (8) and (9), can be written equivalently in terms of the bulk, surface, and curve density fields by recalling Lemma 2.2 and using Identities 2.1. Assuming $\partial S - \partial\Omega = \emptyset$, i.e., the surface S has no boundary within Ω, they include the following local conditions:

$$\operatorname{div}\boldsymbol{\theta}_B^T = \boldsymbol{0} \text{ and } \operatorname{div}\boldsymbol{\alpha}_B^T + ax(\boldsymbol{\theta}_B^T - \boldsymbol{\theta}_B) = \boldsymbol{0} \text{ in } \Omega - S, \tag{10a}$$

$$[\![\boldsymbol{\theta}_B^T]\!]\boldsymbol{n} - \operatorname{div}_S(\boldsymbol{\theta}_S^T) = \boldsymbol{0}, [\![\boldsymbol{\alpha}_B^T]\!]\boldsymbol{n} - \operatorname{div}_S(\boldsymbol{\alpha}_S^T) - ax(\boldsymbol{\theta}_S^T - \boldsymbol{\theta}_S) = \boldsymbol{0},$$
$$\boldsymbol{\theta}_S^T\boldsymbol{n} = \boldsymbol{0}, \text{ and } \boldsymbol{\alpha}_S^T\boldsymbol{n} = \boldsymbol{0} \text{ on } S, \tag{10b}$$

$$\boldsymbol{\theta}_L^T(\boldsymbol{I} - \boldsymbol{t}\otimes\boldsymbol{t}) = \boldsymbol{0},\ \boldsymbol{\alpha}_L^T(\boldsymbol{I} - \boldsymbol{t}\otimes\boldsymbol{t}) = \boldsymbol{0},\ \frac{\partial}{\partial t}(\boldsymbol{\theta}_L^T\boldsymbol{t}) = \boldsymbol{0},$$
$$\text{and } \frac{\partial}{\partial t}(\boldsymbol{\alpha}_L^T\boldsymbol{t}) + ax(\boldsymbol{\theta}_L^T - \boldsymbol{\theta}_L) = \boldsymbol{0} \text{ on } L, \tag{10c}$$

$$\boldsymbol{\theta}_L^T\boldsymbol{t} = \boldsymbol{0} \text{ and } \boldsymbol{\alpha}_L^T\boldsymbol{t} = \boldsymbol{0} \text{ at } \partial L - \partial\Omega, \tag{10d}$$

and the following global conditions:

$$\int_{\partial\Omega_i} \boldsymbol{\theta}_B^T\boldsymbol{n}\,\mathrm{da} + \int_{\partial S\cap\partial\Omega_i} \boldsymbol{\theta}_S^T\boldsymbol{\nu}\,\mathrm{dl} + \boldsymbol{\theta}_L^T\boldsymbol{t}|_{\partial L\cap\partial\Omega_i} = 0 \text{ and} \tag{11a}$$

$$\int_{\partial\Omega_i} \left(\boldsymbol{\alpha}_B^T\boldsymbol{n} + \boldsymbol{x}\times(\boldsymbol{\theta}_B^T\boldsymbol{n})\right)\mathrm{da} + \int_{\partial S\cap\partial\Omega_i} \left(\boldsymbol{\alpha}_S^T\boldsymbol{\nu} + \boldsymbol{x}\times(\boldsymbol{\theta}_S^T\boldsymbol{\nu})\right)\mathrm{dl}$$
$$+ \left(\boldsymbol{\alpha}_L^T\boldsymbol{t} + \boldsymbol{x}\times(\boldsymbol{\theta}_L^T\boldsymbol{t})\right)\Big|_{\partial L\cap\partial\Omega_i} = 0, \tag{11b}$$

each of which represent $k-1$ conditions ($1 \le i \le k-1$) for the domain Ω whose boundary $\partial\Omega$ consists of k mutually disjoint components $\partial\Omega_j$, $0 \le j \le k-1$. The global conditions need to be imposed on any $k-1$, out of k, boundaries. In fact, if the local conditions (10) are satisfied within the domain and the global conditions (11) are satisfied for any $k-1$ boundaries then the global conditions are satisfied for all the k boundaries. Eqs. (10d) hold at those boundaries of the curve L which lie in the interior of Ω; they will not appear if L is a closed loop or if both the boundaries of L lie on $\partial\Omega$ (i.e., when $\partial L - \partial\Omega = \emptyset$). Conditions (10) and (11) are the local and the global conservation laws, respectively, to be satisfied by the bulk, surface, and curve concentrations of the defect densities. The global conditions are topological in the sense that they depend on the overall shape of the domain and are non-trivial only when Ω is non-contractible with $\partial\Omega$ consisting of at least two disjoint components. Examples of such a domain include a hollow ball and a hollow torus. While the former is simply connected the latter is multiply connected. On the other hand, there will be no global conditions for a hollow cylinder which, although being multiply connected, has a single connected boundary. If there are multiple surfaces which intersect a boundary $\partial\Omega_i$ ($i \ne 0$) then the second integral in (11a) and (11b) has to be repeated for each of these surfaces. Similarly, if there are multiple curves which intersect a boundary $\partial\Omega_i$ ($i \ne 0$) then the last term on the left hand side of (11a) and (11b) has to be repeated for each of these curves.

Eqs. $(10c)_{1,2}$ are equivalent to the existence of a pair of smooth vector valued functions on L, $\boldsymbol{\vartheta}$ and $\boldsymbol{b}$, such that

$$\boldsymbol{\theta}_L = \boldsymbol{t}\otimes\boldsymbol{\vartheta} \text{ and } \boldsymbol{\alpha}_L = \boldsymbol{t}\otimes\boldsymbol{b}. \tag{12}$$

According to (10d), a curve of defect concentration cannot end within the domain (unless it ends at a junction where it meets another curve, see Remark 3.1). Furthermore, substituting $(12)_1$ into $(10c)_3$ yields $\boldsymbol{\vartheta}(\boldsymbol{x}) = \boldsymbol{\vartheta}_0$, a constant vector along L. On the other hand, substituting $(12)_2$ into $(10c)_4$ yields $\boldsymbol{b}(\boldsymbol{x}) = \boldsymbol{b}_0 + \boldsymbol{\vartheta}_0\times\boldsymbol{x}$, where $\boldsymbol{b}_0$ is a constant vector along L [6]. Note that $(10c)_{3,4}$, and hence the preceding consequences, do not hold when L coincides with a part of $\partial S - \partial\Omega$ (see Remark 3.2). Therefore, the defect concentrations $\boldsymbol{\theta}_L$ and $\boldsymbol{\alpha}_L$, over a curve $L \subset \Omega$ which does not coincide with an edge of the surface S, can be equivalently described in terms of two constant vectors $\boldsymbol{\vartheta}_0$ and $\boldsymbol{b}_0$ (as is expected from the classical Volterra line defects). Additionally, if $\boldsymbol{\alpha}_L = \boldsymbol{0}$ over any such curve then the disclination is necessarily of a wedge character with a straight defect line L such that $\boldsymbol{\theta}_L = (1/|\boldsymbol{\vartheta}_0|)\boldsymbol{\vartheta}_0\otimes\boldsymbol{\vartheta}_0$. Indeed $\boldsymbol{b} = \boldsymbol{0}$ implies $\boldsymbol{b}_0 + \boldsymbol{\vartheta}_0\times\boldsymbol{x} = \boldsymbol{0}$ which, on differentiating along the curve, imposes $\boldsymbol{\vartheta}_0\times\boldsymbol{t} = \boldsymbol{0}$.

Remark 3.1 (*Intersecting Curves of Defect Concentration*)**.** Consider N regular, oriented, smooth curves $L_n \subset \Omega$ ($1 \le n \le N$), with unit tangent vectors $\boldsymbol{t}_n$, such that they intersect $\partial\Omega$ on one end and meet each other at a common point $O \in \Omega$ at the other end, i.e., $\partial L - \partial\Omega = O$. Let $\boldsymbol{\alpha}_{L_n}$ and $\boldsymbol{\theta}_{L_n}$ denote smooth concentrations of dislocation and disclination fields over the respective curves. Each of these satisfy (10c), in addition to satisfying $\sum_{n=1}^N \boldsymbol{\theta}_{L_n}^T\boldsymbol{t}_n = \boldsymbol{0}$ and $\sum_{n=1}^N \boldsymbol{\alpha}_{L_n}^T\boldsymbol{t}_n = \boldsymbol{0}$ at O. These conditions replace those in (10d) for an isolated curve ending within Ω.

Remark 3.2 ($\partial S - \partial\Omega \ne \emptyset$)**.** Consider a S such that $\partial S - \partial\Omega \ne \emptyset$. Let the oriented curve $\partial S - \partial\Omega$ be denoted by C with unit tangent $\boldsymbol{t}$. In addition to bulk and surface concentrations of defects, as considered above, we also include a smooth concentration of defects (given by $\boldsymbol{\alpha}_C$ and $\boldsymbol{\theta}_C$) over C. Eqs. $(10c)_{1,2}$ and (10d) continue to hold for C (with obvious changes in the notation) while $(10c)_{3,4}$ are replaced by

$$\boldsymbol{\theta}_S^T\boldsymbol{\nu} - \frac{\partial}{\partial t}(\boldsymbol{\theta}_C^T\boldsymbol{t}) = \boldsymbol{0},\ \boldsymbol{\alpha}_S^T\boldsymbol{\nu} - \frac{\partial}{\partial t}(\boldsymbol{\alpha}_C^T\boldsymbol{t}) - ax(\boldsymbol{\theta}_C^T - \boldsymbol{\theta}_C) = \boldsymbol{0} \tag{13}$$

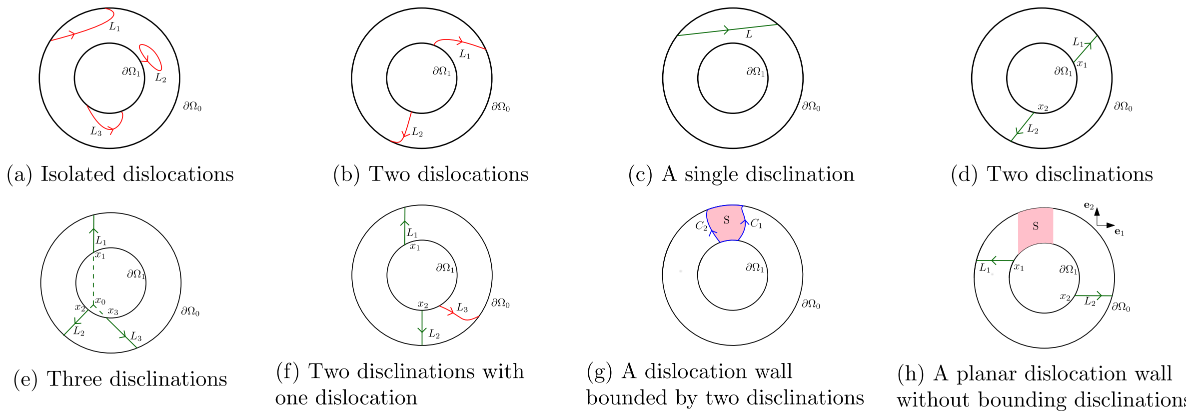
on C, where $\boldsymbol{\nu} = \boldsymbol{n}\times\boldsymbol{t}$.

Remark 3.3 (*Intersecting Surfaces of Defect Concentration*)**.** Consider M regular, oriented, smooth surfaces $S_m \subset \Omega$ ($1 \le m \le M$), with unit normal vectors $\boldsymbol{n}_m$, such that they all meet at a curve $I \subset \Omega$ with unit tangent $\boldsymbol{t}$. Clearly, $I \subset \partial S_m - \partial\Omega$ for all m. Let $\boldsymbol{\alpha}_{S_m}$ and $\boldsymbol{\theta}_{S_m}$ denote smooth concentrations of dislocation and disclination fields over the respective surfaces. Let $\boldsymbol{\alpha}_I$ and $\boldsymbol{\theta}_I$ denote smooth concentrations of dislocation and disclination fields over I. On I, (13) are replaced by $\sum_{m=1}^M \boldsymbol{\theta}_{S_m}^T\boldsymbol{\nu}_m + \frac{\partial}{\partial t}(\boldsymbol{\theta}_I^T\boldsymbol{t}) = \boldsymbol{0}$ and $\sum_{m=1}^M \boldsymbol{\alpha}_{S_m}^T\boldsymbol{\nu}_m + \frac{\partial}{\partial t}(\boldsymbol{\alpha}_I^T\boldsymbol{t}) + ax(\boldsymbol{\theta}_I^T - \boldsymbol{\theta}_I) = \boldsymbol{0}$, where $\boldsymbol{\nu}_m = \boldsymbol{n}_m\times\boldsymbol{t}$.

Remark 3.4 (*Incompatibility, Nilpotency, and Grain Boundary*)**.** We can pose the existence problem (as in Lemma 3.1) in another form involving the incompatibility tensor. For a given distribution of defect densities $\boldsymbol{\Theta} \in \mathcal{D}'(\Omega, \text{Lin})$ and $\boldsymbol{A} \in \mathcal{D}'(\Omega, \text{Lin})$, the existence of distributions $\boldsymbol{K} \in \mathcal{D}'(\Omega, \text{Lin})$ and $\boldsymbol{E} \in \mathcal{D}'(\Omega, \text{Sym})$, satisfying (4), is equivalent to the existence of distributions $\boldsymbol{K} \in \mathcal{D}'(\Omega, \text{Lin})$ and $\boldsymbol{E} \in \mathcal{D}'(\Omega, \text{Sym})$ satisfying $(4)_1$ and $\text{Curl}\,\boldsymbol{\Gamma} + \boldsymbol{\Theta} = \boldsymbol{N}$, where $\boldsymbol{\Gamma} = \boldsymbol{A} - \frac{1}{2}\operatorname{tr}(\boldsymbol{A})\boldsymbol{I}$ is the distributional contortion tensor and $\boldsymbol{N} = \text{Curl}\,\text{Curl}\,\boldsymbol{E}$ is the distributional incompatibility tensor [3]. The verification of this claim is straightforward. The defect density fields are called nilpotent if $\text{Curl}\,\boldsymbol{\Gamma} + \boldsymbol{\Theta} = \boldsymbol{0}$. A special case is that of a grain boundary. Considering the defect densities to be given only in terms of a surface S of dislocation concentration and a curve L of disclination concentration, i.e., $\boldsymbol{A}(\boldsymbol{\phi}) = \int_S \langle\boldsymbol{\alpha}_S, \boldsymbol{\phi}\rangle\,\mathrm{da}$ and $\boldsymbol{\Theta}(\boldsymbol{\phi}) = \int_L \langle\boldsymbol{\theta}_L, \boldsymbol{\phi}\rangle\,\mathrm{dl}$, for $\boldsymbol{\phi} \in \mathcal{D}(\Omega, \text{Lin})$, such that $L = \partial S - \partial\Omega$, we say that these defect densities represent a grain boundary if the associated incompatibility vanishes identically. Writing $\boldsymbol{\Gamma}(\boldsymbol{\phi}) = \int_S \langle\boldsymbol{\gamma}_S, \boldsymbol{\phi}\rangle\,\mathrm{da}$, where $\boldsymbol{\gamma}_S = \boldsymbol{\alpha}_S - \frac{1}{2}\operatorname{tr}(\boldsymbol{\alpha}_S)\boldsymbol{I}$, the nilpotency condition is equivalent to $\boldsymbol{\gamma}_S\times\boldsymbol{n} = \boldsymbol{0}$, $\text{curl}_S\,\boldsymbol{\gamma}_S = \boldsymbol{0}$ on S, and $(\boldsymbol{\gamma}_S\times\boldsymbol{\nu})^T + \boldsymbol{\theta}_L = \boldsymbol{0}$ on $\partial S - \partial\Omega$, where $\boldsymbol{\nu} = \boldsymbol{n}\times\boldsymbol{t}$. Accordingly, we have $\boldsymbol{\gamma}_S = \boldsymbol{\gamma}\otimes\boldsymbol{n}$, where $\boldsymbol{\gamma}$ is a constant vector (representing the misorientation across the boundary) and $\boldsymbol{\theta}_L = \boldsymbol{t}\otimes\boldsymbol{\gamma}$. Therefore if a grain boundary has an edge within the domain then the edge necessarily has to coincide with a disclination curve. The local and global conservation laws (10) and (11) are identically satisfied for these defect densities.

4. Applications for a hollow ball

In this section we demonstrate the applicability of the global conservation laws (11). Towards this end, we consider a hollow ball and determine the restrictions on certain defect configurations as imposed by the conservation laws. Our results, in fact, hold for any domain which is topologically equivalent to a hollow ball. The consequences for other types of domain, such as a hollow torus, can be derived in an analogous manner. Let $\Omega \subset \mathbb{R}^3$ be a hollow ball, i.e., for any fixed positive scalar $a \in \mathbb{R}^+$, $\Omega = \{(x_1, x_2, x_3) \in \mathbb{R}^3 | a^2 < {x_1}^2 + {x_2}^2 + {x_3}^2 < 1\}$. The boundary $\partial\Omega$ of Ω has two mutually disjoint components, $\partial\Omega_0 =$



(a) Isolated dislocations (b) Two dislocations (c) A single disclination (d) Two disclinations

(e) Three disclinations (f) Two disclinations with one dislocation (g) A dislocation wall bounded by two disclinations (h) A planar dislocation wall without bounding disclinations

Fig. 1. Examples of admissible defect configurations in a hollow ball with two disjoint boundaries $\partial\Omega_0$ and $\partial\Omega_1$. Red curves denote dislocations, green lines denote wedge disclinations, blue curves denote disclinations (of a non-wedge character) and solid pink regions denote a dislocation wall. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

$\{(x_1,x_2,x_3) \in \mathbb{R}^3 | {x_1}^2 + {x_2}^2 + {x_3}^2 = 1\}$ and $\partial\Omega_1 = \{(x_1,x_2,x_3) \in \mathbb{R}^3 | {x_1}^2 + {x_2}^2 + {x_3}^2 = a^2\}$. The thickness $(1-a)$ of the spherical shell is inconsequential for our results which, in particular, will hold true even when the walls are infinitesimally thin.

4.1. Dislocation and disclination curves

We consider N regular, oriented, smooth curves $L_n \subset \Omega$ $(1 \le n \le N)$, with unit tangent vectors $\boldsymbol{t}_n$, such that they intersect nowhere with each other or with any surface of defect concentration (see Remarks 3.1 and 3.2). Let $\boldsymbol{\alpha}_{L_n}$ and $\boldsymbol{\theta}_{L_n}$ denote smooth concentrations of dislocation and disclination fields over the respective curves. Following an earlier discussion (see (12)), each of these defect concentrations necessarily have the form

$$\boldsymbol{\theta}_{L_n} = \boldsymbol{t}_n \otimes \boldsymbol{\vartheta}_{0n} \text{ and } \boldsymbol{\alpha}_{L_n} = \boldsymbol{t}_n \otimes \boldsymbol{b}_n, \tag{14}$$

with $\boldsymbol{b}_n(\boldsymbol{x}) = \boldsymbol{b}_{0n} + \boldsymbol{\vartheta}_{0n} \times \boldsymbol{x}$, where $\boldsymbol{b}_{0n}$ and $\boldsymbol{\vartheta}_{0n}$ are vector valued constants. Each curve can possibly intersect the boundary $\partial\Omega_1$ at zero, one, or two points. Let ξ_n be an indicator function (for the curve L_n) such that $\xi_n = 0$ if L_n intersects $\partial\Omega_1$ at zero or two points and $\xi_n = \pm 1$ if L_n intersects $\partial\Omega_1$ at one point (with the correct sign to capture the orientation of the curve at the point of intersection). In the absence of bulk and surface concentrations of defects, the global conditions (11), when written for multiple curves, are reduced to

$$\sum_{1\le n\le N} \xi_n \boldsymbol{\vartheta}_{0n} = \boldsymbol{0} \text{ and } \sum_{1\le n\le N} \xi_n \left(\hat{\boldsymbol{b}}_n + \boldsymbol{x}_n \times \boldsymbol{\vartheta}_{0n}\right) = \boldsymbol{0}, \tag{15}$$

where $\hat{\boldsymbol{b}}_n$ and $\boldsymbol{x}_n$ are the values of $\boldsymbol{b}_n$ and $\boldsymbol{x}$, respectively, at the point of intersection of curve L_n with the boundary $\partial\Omega_1$.

We interpret (15) under further simplifications. Consider, for instance, a scenario when all the curves are pure dislocations, i.e., $\boldsymbol{\vartheta}_{0n} = \boldsymbol{0}$ for all n. Then, according to (15),

$$\sum_{1\le n\le N} \xi_n \hat{\boldsymbol{b}}_n = \boldsymbol{0}. \tag{16}$$

Therefore, if we have a single dislocation curve in the domain ($N = 1$) then it can either appear as a loop (contained within Ω) or as a curve whose both ends intersect only one of the boundaries, $\partial\Omega_0$ or $\partial\Omega_1$ (see Fig. 1(a)) . However, if there are multiple dislocation curves then they can indeed end on each of the two domain boundaries as a long as the restriction (16) is satisfied (see Fig. 1(b)). It should be noted that the global condition does not put any constraint on the mutual position of the dislocations but only on the nature of their Burgers vector. This is contrary to the case of disclinations, as we discuss next. Consider a scenario where all the defect curves are pure disclinations, i.e., $\boldsymbol{b}_n = \boldsymbol{0}$ for all n. Accordingly, (15) reduces to

$$\sum_{1\le n\le N} \xi_n \boldsymbol{\vartheta}_{0n} = \boldsymbol{0} \text{ and } \sum_{1\le n\le N} \xi_n \left(\boldsymbol{x}_n \times \boldsymbol{\vartheta}_{0n}\right) = \boldsymbol{0}. \tag{17}$$

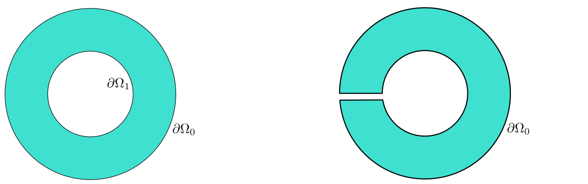
Moreover, as discussed earlier (before Remark 3.1), the disclination curves L_n are necessarily straight with $\boldsymbol{t}_n = (1/|\boldsymbol{\vartheta}_{0n}|)\boldsymbol{\vartheta}_{0n}$. A single disclination line ($N = 1$), cutting through $\partial\Omega_1$, is therefore prohibited (see Fig. 1(c)). If we have two disclinations ($N = 2$), both intersecting $\partial\Omega_1$ at one point, then $\xi_1\boldsymbol{\vartheta}_{01} + \xi_2\boldsymbol{\vartheta}_{02} = \boldsymbol{0}$ and $\xi_1\left(\boldsymbol{x}_1 \times \boldsymbol{\vartheta}_{01}\right) + \xi_2\left(\boldsymbol{x}_2 \times \boldsymbol{\vartheta}_{02}\right) = \boldsymbol{0}$. The former condition is solved by $\xi_1 = -\xi_2 = 1$ and $\boldsymbol{\vartheta}_{01} = \boldsymbol{\vartheta}_{02}$, which essentially implies that $\boldsymbol{\theta}_{L_1} = \boldsymbol{\theta}_{L_2}$. The latter condition is then reduced to $\left(\boldsymbol{x}_1 - \boldsymbol{x}_2\right) \times \boldsymbol{\vartheta}_{01} = \boldsymbol{0}$, which requires the two disclination lines to be collinear (see Fig. 1(d)). If we have three disclinations ($N = 3$), each with one end point on $\partial\Omega_1$, then $(17)_1$ can be satisfied by taking $\xi_1 = \xi_2 = \xi_3 = 1$ (without loss of generality) and $\boldsymbol{\vartheta}_{01} + \boldsymbol{\vartheta}_{02} + \boldsymbol{\vartheta}_{03} = \boldsymbol{0}$. The three disclination lines are therefore coplanar. Condition $(17)_2$, on the other hand, can then be manipulated to write $\boldsymbol{x}_0 \times \boldsymbol{\vartheta}_{01} + \boldsymbol{x}_0 \times \boldsymbol{\vartheta}_{02} + \boldsymbol{x}_3 \times \boldsymbol{\vartheta}_{03} = \boldsymbol{0}$, where $\boldsymbol{x}_0$ is the position of the point where lines L_1 and L_2 meet. Further simplification yields $\left(\boldsymbol{x}_0 - \boldsymbol{x}_3\right) \times \boldsymbol{\vartheta}_{03} = \boldsymbol{0}$. Consequently the three disclination lines are such that they are coplanar and meet at a common point (see Fig. 1(e)). We note that there are no such restrictions on dislocation lines. We consider one final scenario where we take P (out of N) curves to be disclinations and the other $N - P$ $(= Q$, say) curves to be dislocations. Under such circumstances, (15) takes the form $\sum_{1\le n\le P} \xi_n \boldsymbol{\vartheta}_{0n} = \boldsymbol{0}$ and $\sum_{1\le n\le Q} \xi_n \hat{\boldsymbol{b}}_n + \sum_{1\le n\le P} \xi_n \left(\boldsymbol{x}_n \times \boldsymbol{\vartheta}_{0n}\right) = \boldsymbol{0}$. It is now possible to have a single dislocation line ($Q = 1$), intersecting $\partial\Omega_1$ at one point, as long as we have multiple disclination lines in accordance with the above relations. On the other hand, if there are two disclination lines ($P = 2$), each intersecting $\partial\Omega_1$, then they no longer have to be collinear in the presence of appropriate dislocations (see Fig. 1(f)). Of course, if the P disclinations satisfy (17), then the Q dislocations have to necessarily satisfy (16), and vice-versa.

4.2. Dislocation walls and disclination curves

We consider a surface S such that a part of its boundary intersects with $\partial\Omega$ while the other part $\partial S - \partial\Omega$ lies in the interior of Ω. More specifically, the boundary $\partial S - \partial\Omega$ consists of two, mutually disjoint, connected components C_1 and C_2, both intersecting $\partial\Omega_0$ and $\partial\Omega_1$ each at one point (see Fig. 1(g)). We assume a smooth dislocation density concentration $\boldsymbol{\alpha}_S$ over S and smooth disclination density concentrations $\boldsymbol{\theta}_{C_1}$ and $\boldsymbol{\theta}_{C_2}$ over C_1 and C_2, respectively. There are no other defect fields prescribed over the domain. According to $(10c)_{1,2}$ and $(13)_1$, the disclination densities are of the form $\boldsymbol{\theta}_{C_1} = \boldsymbol{t}_1 \otimes \boldsymbol{\vartheta}_{01}$ and $\boldsymbol{\theta}_{C_2} = \boldsymbol{t}_2 \otimes \boldsymbol{\vartheta}_{02}$, where $\boldsymbol{t}_1$ and $\boldsymbol{t}_2$ are unit tangents to the curves C_1 and C_2, respectively, and $\boldsymbol{\vartheta}_{01}, \boldsymbol{\vartheta}_{02}$ are constant vectors. The only non-trivial local conservation laws are those given by $(10b)_{2,4}$ and $(13)_2$, which are reduced to

$$\operatorname{div}_S(\boldsymbol{\alpha}_S^T) = \boldsymbol{0} \text{ and } \boldsymbol{\alpha}_S^T \boldsymbol{n} = \boldsymbol{0} \text{ on } S, \tag{18a}$$

$$\boldsymbol{\alpha}_S^T \boldsymbol{\nu}_1 - \boldsymbol{t}_1 \times \boldsymbol{\vartheta}_{01} = \boldsymbol{0} \text{ on } C_1 \text{ and } \boldsymbol{\alpha}_S^T \boldsymbol{\nu}_2 - \boldsymbol{t}_2 \times \boldsymbol{\vartheta}_{02} = \boldsymbol{0} \text{ on } C_2, \tag{18b}$$



(a) A hollow ball (b) Hollow ball with a cut

Fig. 2. (a) A hollow ball with two disjoint boundaries $\partial\Omega_0$ and $\partial\Omega_1$. (b) A hollow ball with a cut which has only one disjoint boundary $\partial\Omega_0$.

where $\boldsymbol{v}_1 = \boldsymbol{n} \times \boldsymbol{t}_1$ and $\boldsymbol{v}_2 = \boldsymbol{n} \times \boldsymbol{t}_2$. On the other hand, the global conditions (11) require

$$\xi_1 \boldsymbol{\vartheta}_{01} + \xi_2 \boldsymbol{\vartheta}_{02} = 0 \text{ and} \tag{19a}$$

$$\int_{\partial S \cap \partial\Omega_1} \boldsymbol{\alpha}_S^T \boldsymbol{v}\, \mathrm{dl} + \xi_1 (\boldsymbol{x}_1 \times \boldsymbol{\vartheta}_{01}) + \xi_2 (\boldsymbol{x}_2 \times \boldsymbol{\vartheta}_{02}) = 0, \tag{19b}$$

where ξ_2 and ξ_2 are as defined in the previous subsection. According to $(18b)_1$, if $\boldsymbol{\alpha}_S^T \boldsymbol{v}_1 \neq \boldsymbol{0}$ then the edge C_1 is necessarily a disclination of a non-wedge character (and hence not necessarily straight). However, if $\boldsymbol{\alpha}_S^T \boldsymbol{v}_1 = \boldsymbol{0}$ then the edge C_1 need not support a disclination; if it does, then it has to be a wedge disclination and C_1 has to be straight. We illustrate this with a simple example. Consider S to be planar ($\boldsymbol{n} = \boldsymbol{e}_3$) such that two of its edges coincide with $\partial\Omega$ and the other two lie within Ω such that $\boldsymbol{v}_1 = -\boldsymbol{e}_1$ and $\boldsymbol{v}_2 = \boldsymbol{e}_1$ (see Fig. 1(h)). We assume $\boldsymbol{\alpha}_S = \boldsymbol{e}_2 \otimes \boldsymbol{b}_0$, where $\boldsymbol{b}_0$ is a constant vector. Consequently (18a) are identically satisfied. Moreover, (18b) are also satisfied if we assume vanishing disclinations at the interior edges C_1 and C_2. Finally, the global equation (11b) can be satisfied by considering two isolated disclinations away from the dislocation wall, with the same Frank vector, but not collinear (see Fig. 1(h)). This situation is similar to that of Fig. 1(f) where the non-collinearity of the two disclination lines is balanced by a single dislocation.

4.3. Bulk defect densities

We consider defect fields over Ω to be given in terms of a bulk dislocation density $\boldsymbol{\alpha}_B \in C^\infty(\Omega, \mathrm{Lin})$ and a bulk disclination density $\boldsymbol{\theta}_B \in C^\infty(\Omega, \mathrm{Lin})$. There are no other defect densities. The classical continuum theory of defects [4] is formulated within such a framework. According to the discussion in Section 3, the following local and global conditions (derivable from (10) and (11))

$$\operatorname{div} \boldsymbol{\theta}_B^T = \boldsymbol{0} \text{ and } \operatorname{div} \boldsymbol{\alpha}_B^T + ax(\boldsymbol{\theta}_B^T - \boldsymbol{\theta}_B) = \boldsymbol{0} \text{ in } \Omega, \tag{20a}$$

$$\int_{\partial\Omega_1} \boldsymbol{\theta}_B^T \boldsymbol{n}\, \mathrm{da} = \boldsymbol{0} \text{ and } \int_{\partial\Omega_1} \left(\boldsymbol{\alpha}_B^T \boldsymbol{n} + \boldsymbol{x} \times (\boldsymbol{\theta}_B^T \boldsymbol{n})\right) \mathrm{da} = \boldsymbol{0} \tag{20b}$$

are necessary and sufficient for there to exist a strain field $\boldsymbol{\epsilon} \in C^\infty(\Omega, \mathrm{Sym})$ and a bend-twist field $\boldsymbol{\kappa} \in C^\infty(\Omega, \mathrm{Lin})$ such that $\boldsymbol{\theta}_B = \operatorname{curl} \boldsymbol{\kappa}^T$ and $\boldsymbol{\alpha}_B = \operatorname{curl} \boldsymbol{\epsilon} + \operatorname{tr}(\boldsymbol{\kappa})\boldsymbol{I} - \boldsymbol{\kappa}^T$. We first restrict ourselves to the case when $\boldsymbol{\theta}_B = \boldsymbol{0}$. The preceding result can be recast as follows. The equations

$$\operatorname{div} \boldsymbol{\alpha}_B^T = \boldsymbol{0} \text{ in } \Omega \text{ and } \int_{\partial\Omega_1} \boldsymbol{\alpha}_B^T \boldsymbol{n}\, \mathrm{da} = \boldsymbol{0} \tag{21}$$

are necessary and sufficient for there to exist a distortion field $\boldsymbol{\beta} \in C^\infty(\Omega, \mathrm{Lin})$ such that $\boldsymbol{\alpha}_B = \operatorname{curl} \boldsymbol{\beta}$. The dislocation density field $\boldsymbol{\alpha}_B = (\boldsymbol{e}_r \otimes \boldsymbol{b})/r^2$, where r is the radial coordinate ($r^2 = x_1^2 + x_2^2 + x_3^2$) and $\boldsymbol{b}$ is a constant vector, satisfies $(21)_1$ but not $(21)_2$. It is therefore an admissible dislocation density field for a contractible domain (as long as the origin lies outside the domain), such as the one shown in Fig. 2(b), but not for a hollow ball. Analogously, for the case with $\boldsymbol{\alpha}_B = \boldsymbol{0}$, the equations

$$\operatorname{div} \boldsymbol{\theta}_B^T = \boldsymbol{0} \text{ and } ax(\boldsymbol{\theta}_B^T - \boldsymbol{\theta}_B) = \boldsymbol{0} \text{ in } \Omega, \tag{22a}$$

$$\int_{\partial\Omega_1} \boldsymbol{\theta}_B^T \boldsymbol{n}\, \mathrm{da} = \boldsymbol{0} \text{ and } \int_{\partial\Omega_1} \left(\boldsymbol{x} \times (\boldsymbol{\theta}_B^T \boldsymbol{n})\right) \mathrm{da} = \boldsymbol{0} \tag{22b}$$

are necessary and sufficient for there to exist a strain field $\boldsymbol{\epsilon} \in C^\infty(\Omega, \mathrm{Sym})$ such that $\boldsymbol{\theta}_B = \operatorname{curl}\operatorname{curl} \boldsymbol{\epsilon}$. The field $\boldsymbol{\theta}_B = (\langle \boldsymbol{p}, \boldsymbol{e}_r \rangle \boldsymbol{e}_r \otimes \boldsymbol{e}_r + \boldsymbol{p} \otimes \boldsymbol{e}_r + \boldsymbol{e}_r \otimes \boldsymbol{p} - \langle \boldsymbol{p}, \boldsymbol{e}_r \rangle \boldsymbol{I})/r^2$, where $\boldsymbol{p}$ is a constant vector, satisfies (22a) but not (22b). It is therefore an admissible disclination density field for a contractible domain (as long as the origin lies outside the domain), such as the one shown in Fig. 2(b), but not for a hollow ball.

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Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Supplementary data

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.mechrescom.2021.103806.

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