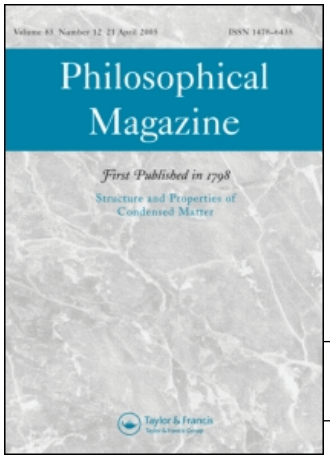

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Shaofan Li [a]
[a] Department of Civil and Environmental Engineering, University of California, Berkeley, CA94720, USA

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On variational symmetry of defect potentials and multiscale configurational force

Shaofan Li*

Department of Civil and Environmental Engineering, University of California, Berkeley, CA94720, USA

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In this work, we study invariant properties of defect potentials that are capable of describing defect motions in a continuum. By formulating two canonical defect theories, a generalized Nye theory and the Kröner–de Wit theory, we have found three defect potentials that are variational, i.e. their associated Euler–Lagrange equations are differential compatibility conditions of the continuum and defects. Consequently, symmetry properties of these variational functionals render several classes of new conservation laws and invariant integrals that are related with continuum compatibility conditions, which are independent of the constitutive relations of the continuum. The contour integral of the corresponding conserved quantity is path-independent, if the domain encompassed by such an integral is specifically defect-free. The invariant integral is applied to study macroscopically brittle fracture, and a *multiscale Griffith criterion* is proposed, which leads to a rigorous justification of the well-known Griffith–Irwin theory.

Keywords: compatibility; conservation laws; configurational force; dislocation; fracture; multiscale analysis; path-independent integral

1. Introduction

It is well established today that the mathematical structure of the configurational force is the conservation law of continuum mechanics, which is based on Noether's invariant theory, e.g. [1,2], and the physical origin of the configurational force is from the balance law of continuum thermodynamics, e.g. [3], which is a manifestation of the symmetry properties of the free-energy density. The configurational force that we refer to is a material force acting on defects in the sense of Eshelby [4,5], which has been eloquently elaborated in several monographs [6–9].

However, classical elasticity, both linear and finite deformation theories, does not have an intrinsic length-scale. Therefore, in the realm of classical elasticity, the configurational mechanics do not have a multiscale character, which is in contrast or in conflict with physical reality where defects and the effects of defect evolutions are multiscale in nature. To bring the length-scale into configurational mechanics, some workers have explored the multiscale paradigm of Gauge theory (e.g. [10–13]), and others have studied symmetry

*Email: shaofan@berkeley.edu

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properties of the free-energy with strain gradient contribution, e.g. [14–17]. The latter requires materials exhibiting strong strain gradient effects, which may not be as common as we thought before as recent evidence suggests, e.g. [18].

In conventional continuum mechanics, the motion of the continuum is governed by both force equilibrium and compatibility conditions, whereas in configurational mechanics, defect motions are only subjected to material force without considering any kinematic constraints. To fix this imbalance, Li et al. [19] proposed a concept of *configurational compatibility* in the hope of finding additional governing equations for defect motions by combining the *defect equilibrium approach* and the *defect compatibility approach*. The present work is concerned with two other aspects: (1) variational symmetry of defect potentials; Li et al. [19] only discusses one particular defect potential, which may not even be variationally meaningful; as will be shown in this work, there are other distinct types of defect potentials depending on the types of defects, for instance dislocations or disclinations; (2) to explore the possibility of a multiscale configurational mechanics.

In this paper, we shall systematically study invariant (symmetry) properties of defect potentials by exploring their links to configurational compatibility and multiscale configurational forces, and we shall apply them to study brittle fracture. The presentation is organized into five sections. We start in Section 2 with the construction of various defect potentials based on the linear continuum theory of dislocations. By utilizing these defect potentials, new classes of compatibility conservation laws are derived in Section 3 by applying Noether's theorems [1,20]. In Section 4, we apply one of the compatibility–momentum tensors to formulate a multiscale energy–momentum tensor and to study brittle fracture. A multiscale Griffith criterion is proposed. We close the presentation in Section 5 with a few remarks.

2. Variational defect potentials

In order to study variational symmetry of defect potentials, we first proceed to identify variationally meaningful defect potentials, by which we mean that a defect potential will provide differential compatibility equations in a variational statement such as its Euler–Lagrange equations. We refer to such a defect potential as the *variational defect potential*. For the sake of a self-contained presentation, we start by reviewing the continuum theory of dislocations.

2.1. *The linear continuum theory of dislocations*

To fix the notation, we first introduce the convention used in the continuum description of defects. We identify a perfectly ordered state as a defect-free state. Considering dislocations as the main defect in this work, we incorporate plasticity into the continuum model as the manifestation of the dislocation ensemble state, which is achieved by decomposing the total strain field ϵ of the solid into an elastic part ϵ^e, which gives rise to stresses based on the general assumptions of elasticity theory, and a plastic or inelastic part ϵ^p, which changes the shape of the solid and leads to permanent deformation. In the infinitesimal case, this decomposition is given as

$$\boldsymbol{\epsilon} = \boldsymbol{\epsilon}^e + \boldsymbol{\epsilon}^p. \tag{1}$$

Contrary to $\boldsymbol{\epsilon}$, which is always a compatible field, $\boldsymbol{\epsilon}^e$ and $\boldsymbol{\epsilon}^p$ are, in general, not compatible fields. Since plastic deformation is permanent, the elastic strain $\boldsymbol{\epsilon}^e$ no longer satisfies the compatibility equations, which will be commensurate with defect distributions that constitute inelastic deformations. Thus the continuum defect theory can be formulated with elastic or inelastic kinematic variables that represent the defect distribution. In order to describe a defect state, one uses other kinematic variables. For example, the curvature, which may serve as another state quantity, plays a dominant role in the continuum theory of defects, as will be shown below. Following [21,22], we introduce the corresponding anti-symmetric rotation tensors $\boldsymbol{\omega}, \boldsymbol{\omega}^e, \boldsymbol{\omega}^p$, and distortion tensors $\boldsymbol{\beta}, \boldsymbol{\beta}^e, \boldsymbol{\beta}^p$ as

$$\boldsymbol{\beta} = \boldsymbol{\epsilon} + \boldsymbol{\omega}, \quad \boldsymbol{\beta}^e = \boldsymbol{\epsilon}^e + \boldsymbol{\omega}^e \quad \text{and} \quad \boldsymbol{\beta}^p = \boldsymbol{\epsilon}^p + \boldsymbol{\omega}^p, \tag{2}$$

with the analogous decomposition as (1), namely

$$\boldsymbol{\omega} = \boldsymbol{\omega}^e + \boldsymbol{\omega}^p \quad \text{and} \quad \boldsymbol{\beta} = \boldsymbol{\beta}^e + \boldsymbol{\beta}^p \tag{3}$$

and

$$\boldsymbol{\beta} := \nabla \otimes \mathbf{u}, \quad \boldsymbol{\epsilon} = \frac{1}{2}(\boldsymbol{\beta} + \boldsymbol{\beta}^T), \quad \text{and} \quad \boldsymbol{\omega} = \frac{1}{2}(\boldsymbol{\beta} - \boldsymbol{\beta}^T) \tag{4}$$

where $\mathbf{u}$ is the total displacement field. Note that the infinitesimal rotation tensor, $\boldsymbol{\omega}$, defined in this paper differs by a minus sign from the conventional definition of the infinitesimal rotation in the literature.

Remark 2.1: In this paper, we mainly use Cartesian tensors. To conform with the notation of the existing literature on continuum dislocations, especially [21,22], we adopt the following conventions on gradient and divergence operators,

$$\nabla \otimes \mathbf{u} := \frac{\partial u_j}{\partial x_i}\mathbf{e}_i \otimes \mathbf{e}_j = \partial_i u_j \mathbf{e}_i \otimes \mathbf{e}_j = u_{j,i}\mathbf{e}_i \otimes \mathbf{e}_j, \quad \text{and} \quad \nabla \cdot \mathbf{A} = A_{ij,i}\mathbf{e}_j \tag{5}$$

where $\mathbf{e}_i$, $i = 1, 2, 3$ are the basis vectors in Cartesian coordinate, and $\mathbf{A} = A_{ij}\mathbf{e}_i \otimes \mathbf{e}_j$ represents an arbitrary differentiable second-order tensor. Please note the subtle difference between this convention and the convention used in many mathematics reference books. Consequently, the Divergence Theorem reads as

$$\int_\Omega \nabla \cdot \mathbf{A}\, \mathrm{d}\Omega = \int_{\partial\Omega} \mathbf{n} \cdot \mathbf{A} \mathrm{d}S, \quad \text{or} \quad \int_\Omega A_{k\alpha,k}\, \mathrm{d}\Omega = \int_{\partial\Omega} A_{k\alpha} n_k \mathrm{d}S. \tag{6}$$

In order to describe how a body is deformed by the total distortion $\boldsymbol{\beta}$, we may write the change of the total displacement vector

$$\mathbf{du} = \mathbf{dx} \cdot \boldsymbol{\beta} \quad \text{or} \quad \mathrm{d}u_j = \beta_{ij}\mathrm{d}x_i. \tag{7}$$

The term 'distortion' is used instead of displacement gradient, because the $\boldsymbol{\beta}$'s are gradients as in (7) only if the corresponding deformation is compatible. This is the case for the total distortion but in general does not hold for either elastic or plastic distortion.

To describe the defect, we define the *geometrically necessary dislocation density* according to [23] in terms of the plastic distortion

$$\mathbf{d}^{\mathrm{GND}} := \nabla \times \boldsymbol{\beta}^p, \text{ or in component form } d_{ij}^{\mathrm{GND}} = e_{ik\ell}\partial_k \beta_{\ell j}^p = e_{ik\ell}\beta_{\ell j,k}^p \tag{8}$$

where the permutation symbol $e_{ik\ell}$ is used. Since the total distortion $\beta_{\ell j}^t$ has to remain compatible, namely $e_{ik\ell}\beta_{\ell j,k}^t = 0$, which means that the body is not allowed to break, we can rewrite (8) as

$$\boldsymbol{\alpha} := -\nabla \times \boldsymbol{\beta}^e = \mathbf{d}^{\mathrm{GND}}. \tag{9}$$

As pointed out in [22], the second equality in (9) is no longer a definition; it is a physical law. In this paper, we use $\boldsymbol{\alpha}$ to represent the curl of the negative elastic distortion, and the compatibility law is: $\boldsymbol{\alpha} = \mathbf{d}^{\mathrm{GND}}$.

The condition of conservation of the Burgers vector follows directly from (9) as

$$\nabla \cdot \boldsymbol{\alpha} = 0, \tag{10}$$

which implies that dislocations do not end inside the body. The physical interpretation of (10) is the conservation or the balance of the net Burgers vector because

$$\oint_S \mathbf{n} \cdot \boldsymbol{\alpha} \mathrm{d}S = \mathbf{b}, \tag{11}$$

where $\mathbf{b}$ is the Burgers vector, and the net Burgers vector for a closed contour integral inside the body has to be zero.

As usual we can express an anti-symmetric tensor by its axial (rotation) vector

$$\boldsymbol{\omega}^e = \boldsymbol{\mathcal{E}} : \boldsymbol{\theta}\left(\omega_{ij}^e = e_{ijk}\theta_k\right) \quad \text{or} \quad \boldsymbol{\theta} = \frac{1}{2}\boldsymbol{\mathcal{E}} : \boldsymbol{\omega}^e\left(\theta_k = \frac{1}{2}e_{ijk}\omega_{ij}^e\right), \tag{12}$$

where $\boldsymbol{\mathcal{E}} := e_{ijk}\,\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k$ is the alternating tensor, e_{ijk} is the permutation symbol, and $\boldsymbol{\theta}_k$ is the axial vector of elastic rotation ω_{ij}^e. By virtue of (12), we can further write

$$e_{ik\ell}\omega_{\ell j,k}^e = e_{ik\ell}e_{\ell jm}\theta_{m,k} = \theta_{k,k}\delta_{ij} - \theta_{i,j}, \tag{13}$$

where the Kronecker symbol δ_{ij} is used. Now we can use (2), (9), and (13) to express the geometrically necessary dislocation density in terms of the elastic strain and elastic rotation

$$\alpha_{ij} = -e_{ik\ell}\epsilon_{\ell j,k}^e + \theta_{i,j} - \theta_{k,k}\delta_{ij}. \tag{14}$$

If we introduce the curvature $\boldsymbol{\kappa}$ and the curl of the elastic strain $\boldsymbol{\zeta}$ as

$$\boldsymbol{\kappa} := \nabla \otimes \boldsymbol{\theta} \tag{15}$$

and

$$\boldsymbol{\zeta} := \nabla \times \boldsymbol{\epsilon}^e, \tag{16}$$

we can rewrite (14) as

$$\alpha_{ij} = -\zeta_{ij} + \kappa_{ji} - \kappa_{kk}\delta_{ij}. \tag{17}$$

Because $\epsilon^e_{\ell i} = \epsilon^e_{i\ell}$, $\zeta_{ii} = e_{ik\ell}\epsilon^e_{\ell i,k} \equiv 0$. We can link the trace of the curvature κ_{kk} with the trace of the geometrically necessary dislocation density α_{kk} as $\kappa_{kk} = -(1/2)\alpha_{kk}$, which further allows us to write the inverse relation of (17) as

$$\kappa_{ij} = \zeta_{ji} + \alpha_{ji} - \frac{1}{2}\alpha_{kk}\delta_{ij}. \tag{18}$$

Summarizing (17) and (18), we have the following set of kinematic relations,

$$\boldsymbol{\alpha} = -\boldsymbol{\zeta} + \boldsymbol{\kappa}^T - \mathrm{tr}(\boldsymbol{\kappa})\mathbb{I}^{(2)} \quad \text{and} \quad \boldsymbol{\kappa} = \boldsymbol{\zeta}^T + \boldsymbol{\alpha}^T - \frac{1}{2}\mathrm{tr}(\boldsymbol{\alpha})\mathbb{I}^{(2)} \tag{19}$$

where $\mathbb{I}^{(2)}$ is the second-order unit tensor, and tr is the trace operator.

Nye [23] made an approximation to (19) by neglecting the contribution from the curl of the elastic strain $\boldsymbol{\zeta}$, which is only valid for small elastic strain gradients. This allows us to approximate (19) as

$$\boldsymbol{\alpha} = \mathbb{P} : \boldsymbol{\kappa} \quad \text{and} \quad \boldsymbol{\kappa} = \mathbb{Q} : \boldsymbol{\alpha}, \tag{20}$$

where we introduce the tensors $\mathbb{P}$ and $\mathbb{Q}$ given as

$$\mathbb{P} = \mathbb{I}^T - \mathbb{I}^{(2)} \otimes \mathbb{I}^{(2)}, \quad \text{and} \quad \mathbb{Q} = \mathbb{I}^T - \frac{1}{2}\mathbb{I}^{(2)} \otimes \mathbb{I}^{(2)} \tag{21}$$

where $\mathbb{I}^{(2)} = \delta_{ij}\,\mathbf{e}_i \otimes \mathbf{e}_j$ is the second-order unit tensor, and

$$\mathbb{I}^T := \delta_{i\ell}\delta_{jk}\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_\ell \tag{22}$$

is a fourth order tensor that maps any second-order tensor, $\mathbf{A}$, to its transport, i.e.

$$\mathbf{A}^T = \mathbb{I}^T : \mathbf{A}.$$

Moreover $\mathbb{P} : \mathbb{Q} = \mathbb{I}$ where

$$\mathbb{I} = \delta_{ik}\delta_{j\ell}\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_\ell$$

is the fourth-order unit tensor.

In passing, we note that both $\mathbb{P}$ and $\mathbb{Q}$ have major symmetry, i.e.

$$\mathbb{P}_{ijk\ell} = \mathbb{P}_{k\ell ij} \quad \text{and} \quad \mathbb{Q}_{ijk\ell} = \mathbb{Q}_{k\ell ij},$$

and they do not have minor symmetry, i.e.

$$\mathbb{P}_{ijk\ell} \neq \mathbb{P}_{jik\ell} \neq \mathbb{P}_{ji\ell k} \quad \text{and} \quad \mathbb{Q}_{ijk\ell} \neq \mathbb{Q}_{jik\ell} \neq \mathbb{Q}_{ji\ell k}.$$

Alternatively one may write (20) as

$$\boldsymbol{\alpha}^T = \mathbb{S} : \boldsymbol{\kappa}, \quad \boldsymbol{\kappa} = \mathbb{T} : \boldsymbol{\alpha}^T; \quad \text{or} \quad \boldsymbol{\alpha} = \mathbb{S} : \boldsymbol{\kappa}^T, \quad \boldsymbol{\kappa}^T = \mathbb{T} : \boldsymbol{\alpha}, \tag{23}$$

where we introduce the tensors $\mathbb{S}$ and $\mathbb{T}$ defined as

$$\mathbb{S} = \mathbb{I} - \mathbb{I}^{(2)} \otimes \mathbb{I}^{(2)}, \quad \text{and} \quad \mathbb{T} = \mathbb{I} - \frac{1}{2}\mathbb{I}^{(2)} \otimes \mathbb{I}^{(2)} \tag{24}$$

and $\mathbb{S}:\mathbb{T}=\mathbb{I}$. Similarly, both $\mathbb{S}$ and $\mathbb{T}$ have major symmetry, i.e.

$$\mathbb{S}_{ijk\ell}=\mathbb{S}_{k\ell ij} \quad \text{and} \quad \mathbb{T}_{ijk\ell}=\mathbb{T}_{k\ell ij},$$

but not minor symmetry, i.e.

$$\mathbb{S}_{ijk\ell}\neq\mathbb{S}_{jik\ell}\neq\mathbb{S}_{ji\ell k} \quad \text{and} \quad \mathbb{T}_{ijk\ell}\neq\mathbb{T}_{jik\ell}\neq\mathbb{T}_{ji\ell k}.$$

Remark 2.2: **(a)** All mapping tensors are not projection tensors. In fact, it is easy to verify that

$$\begin{aligned}\mathbb{P}:\mathbb{P}&=\mathbb{S}+2\mathbb{I}^{(2)}\otimes\mathbb{I}^{(2)}, \quad \text{and} \quad \mathbb{Q}:\mathbb{Q}=\mathbb{T}+\frac{1}{4}\mathbb{I}^{(2)}\otimes\mathbb{I}^{(2)}.\\ \mathbb{S}:\mathbb{S}&=\mathbb{S}+2\mathbb{I}^{(2)}\otimes\mathbb{I}^{(2)}, \quad \text{and} \quad \mathbb{T}:\mathbb{T}=\mathbb{T}+\frac{1}{4}\mathbb{I}^{(2)}\otimes\mathbb{I}^{(2)}.\end{aligned} \tag{25}$$

(b) All mapping tensors, $\mathbb{P}$, $\mathbb{Q}$, $\mathbb{S}$ and $\mathbb{T}$, are indefinite, i.e. they are neither positive definite nor negative definite.

The beauty of Nye's theory is that it is a canonical defect theory in the sense that it only depends on two kinematic state variables, and the two kinematic state variables are related to each other (see (20)), so one can define a defect potential such as

$$W^{(N)}(\boldsymbol{\alpha})=\frac{1}{2}\boldsymbol{\alpha}:\boldsymbol{\kappa}=\frac{1}{2}\boldsymbol{\alpha}:\mathbb{Q}:\boldsymbol{\alpha}=\frac{1}{2}\boldsymbol{\kappa}:\mathbb{P}:\boldsymbol{\kappa}. \tag{26}$$

However, the weakness of Nye's theory is that it is an approximate theory. We show next that without the approximation made in [23], i.e. without neglecting the contribution from the curl of elastic strains, we can still reduce (19) to a canonical form.

(I) The generalized Nye theory: Combining $\boldsymbol{\alpha}$ and $\boldsymbol{\zeta}$: We can combine the geometrically necessary dislocation density $\boldsymbol{\alpha}$ with the curl of the elastic strains $\boldsymbol{\zeta}$ to define a new geometric object $\boldsymbol{\gamma}$ as

$$\boldsymbol{\gamma}:=\boldsymbol{\zeta}+\boldsymbol{\alpha}. \tag{27}$$

Equation (2) allows us to write this new object as the curl of elastic rotations if $\boldsymbol{\alpha}=-\nabla\times\boldsymbol{\beta}^e$,

$$\boldsymbol{\gamma}=-\nabla\times\boldsymbol{\omega}^e. \tag{28}$$

Since the divergence of the geometrically necessary dislocation density $\boldsymbol{\alpha}_{ij}$ vanishes by (10) and partial derivatives commute, one can immediately find the following governing equation for the defined quantity:

$$\nabla\cdot\boldsymbol{\gamma}=0. \tag{29}$$

Substituting (27) into (19) and using the fact that $\boldsymbol{\zeta}_{kk}=0$ we obtain $\boldsymbol{\gamma}_{kk}=\boldsymbol{\alpha}_{kk}$, and we find that the relation between the negative curl of elastic rotations, $\boldsymbol{\gamma}$, and the curvature tensor, $\boldsymbol{\kappa}$, is given by

$$\begin{aligned}\boldsymbol{\gamma} &= \mathbb{P}:\boldsymbol{\kappa}, \quad \text{or} \quad \boldsymbol{\gamma}^T=\mathbb{S}:\boldsymbol{\kappa};\\ \boldsymbol{\kappa} &= \mathbb{Q}:\boldsymbol{\gamma}, \quad \text{or} \quad \boldsymbol{\kappa}^T=\mathbb{T}:\boldsymbol{\gamma};\end{aligned} \tag{30}$$

in terms of the tensors $\mathbb{P}$ and $\mathbb{Q}$ or the tensors $\mathbb{S}$ and $\mathbb{T}$. When $\boldsymbol{\zeta}=0$, Equations (30) degenerate to the original Nye relation in terms of the geometrically necessary dislocation density, $\boldsymbol{\alpha}$, and the curvature tensor, $\boldsymbol{\kappa}$, given in (20). This recombination of kinematic variables enables us to construct defect potentials solely based on either elastic rotation, $\boldsymbol{\omega}^e$, or its axial vector, $\boldsymbol{\theta}$. We call this combination the *generalized Nye theory*.

Remark 2.3: The divergence-free identity (29) holds true for

$$\nabla\cdot\boldsymbol{\alpha}=0,\quad \text{and}\quad \nabla\cdot\boldsymbol{\zeta}=0 \tag{31}$$

because in the absence of disclinations,

$$\boldsymbol{\alpha}=-\nabla\times\boldsymbol{\beta}^e, \tag{32}$$

and it is always true that $\boldsymbol{\zeta}:=\nabla\times\boldsymbol{\epsilon}^e$. If there is a disclination distribution, the first equality, or definition, of (9) will no longer be valid, instead

$$\boldsymbol{\alpha}=\tilde{\boldsymbol{\alpha}}-\nabla\times\boldsymbol{\beta}^e,\quad \tilde{\boldsymbol{\alpha}}=\tilde{\boldsymbol{\kappa}}^T-\mathrm{tr}(\tilde{\boldsymbol{\kappa}})\mathbb{I}^{(2)},\quad \text{and}\quad \boldsymbol{\kappa}=\tilde{\boldsymbol{\kappa}}+\nabla\otimes\boldsymbol{\theta} \tag{33}$$

where the additional curvature $\tilde{\boldsymbol{\kappa}}$ is induced by disclination distributions.

In one of the disclination theories, i.e. [24,25], one can determine $\tilde{\boldsymbol{\kappa}}$ by the disclination distribution density, $\boldsymbol{\psi}$, through a differential relation, i.e.

$$\boldsymbol{\psi}=\frac{1}{2}\boldsymbol{\mathcal{E}}:\boldsymbol{\xi},\quad \text{and}\quad \boldsymbol{\xi}=-\nabla\times\tilde{\boldsymbol{\kappa}}. \tag{34}$$

The dislocation continuity equation under the combined dislocation and disclination distributions will become

$$\nabla\cdot\boldsymbol{\alpha}+2\boldsymbol{\psi}=0\quad \text{or}\quad \nabla\cdot\boldsymbol{\gamma}+2\boldsymbol{\psi}=0. \tag{35}$$

An interpretation of Equation (35) is that in the presence of disclinations the Burgers vector is no longer conserved.

(II) The Kröner–de Wit theory: Combining $\boldsymbol{\kappa}$ and $\boldsymbol{\zeta}$: Another way to achieve a canonical defect theory is by combining the curvature tensor, $\boldsymbol{\kappa}$, with the curl of elastic strains, $\boldsymbol{\zeta}$, to define a new geometric object, the contortion $\mathbf{K}$, as

$$\mathbf{K}:=\boldsymbol{\kappa}-\boldsymbol{\zeta}^T. \tag{36}$$

Substituting (36) into (19) and using the fact that the trace $\boldsymbol{\zeta}_{ii}\equiv 0$ and therefore $K_{ii}=\boldsymbol{\kappa}_{ii}$, we find that the relation between the geometrically necessary dislocation density $\boldsymbol{\alpha}$ and the contortion $\mathbf{K}$ is given as

$$\begin{aligned}\boldsymbol{\alpha}&=\mathbb{P}:\mathbf{K},\quad \text{or}\quad \boldsymbol{\alpha}^T=\mathbb{S}:\mathbf{K},\\ \mathbf{K}&=\mathbb{Q}:\boldsymbol{\alpha},\quad \text{or}\quad \mathbf{K}^T=\mathbb{T}:\boldsymbol{\alpha}.\end{aligned} \tag{37}$$

Again the kinematic field variables are related with each other in terms of the tensors $\mathbb{P}$ and $\mathbb{Q}$ introduced in (21). When $\boldsymbol{\zeta}=0$, Equations (37) degenerate to the original Nye relations in terms of the geometrically necessary dislocation density, $\boldsymbol{\alpha}$, and the curvature tensor, $\boldsymbol{\kappa}$, given in (20). This recombination of the kinematic variables provides a basis for constructing defect potentials solely dependent on a single state variable – either

Table 1. Kinematic field quantities describing distributed dislocations.

Field	$\boldsymbol{\alpha}$	$\boldsymbol{\zeta}$	$\boldsymbol{\gamma}$	$\boldsymbol{\theta}$
β^e	$-\nabla\times\boldsymbol{\beta}^e$			
$\boldsymbol{\epsilon}^e$		$\nabla\times\boldsymbol{\epsilon}^e$		
$\boldsymbol{\omega}^e$			$-\nabla\times\boldsymbol{\omega}^e$	$(1/2)\boldsymbol{\mathcal{E}}:\boldsymbol{\omega}^e$
$\boldsymbol{\kappa}$	$-\boldsymbol{\zeta}+\mathbb{P}:\boldsymbol{\kappa}$	$-\boldsymbol{\alpha}+\mathbb{P}:\boldsymbol{\kappa}$	$\mathbb{P}:\boldsymbol{\kappa}$	$\nabla\otimes\boldsymbol{\theta}$
$\boldsymbol{K}$	$\mathbb{P}:\mathbf{K}$	$\boldsymbol{\kappa}^T-\mathbf{K}^T$		

elastic distortion, $\boldsymbol{\beta}^e$, or elastic strain $\boldsymbol{\epsilon}^e$. We term this recombination of kinematic variables the Kröner–de Wit theory.

Remark 2.4: A similar quantity to the curl of elastic strains $\boldsymbol{\zeta}$ has been used in [26]. Contrary to our definition of $\boldsymbol{\zeta}=\nabla\times\boldsymbol{\epsilon}^e$ in (16) in terms of elastic strains, in [26] the total strain has been used. In [27] a quantity identical to $\boldsymbol{\gamma}$ in (27) has been derived by linearization of the geometrically necessary dislocation density in a rigid plastic material, i.e. a material with vanishing elastic strains. Therefore we can also view $\boldsymbol{\gamma}$ as a measure of the dislocation density.

For easy reference, in Table 1, we summarize all the relationships among the kinematic variable fields that are used to describe defect distributions.

2.2. *Variational defect potentials*

We now define the *variational defect potential*. There are two criteria about this definition: (1) the potential solely consists of kinematics variables that are used to measure defect distributions, and (2) the Euler–Lagrange equation resulted from the defect potential functional is a physical law or a physically meaningful 'balance law', such as the integrability condition of strains or the conservation of a defect variable. In short, the variational defect potential provides an action functional density for a variational principle that can yield kinematic compatibility conditions in a continuum.

Obviously, not all defect potentials are variationally meaningful. Next we shall screen all possible defect potentials to identity which are the variational defect potentials. Depending on whether the defect potential depends on a vectorial field such as the rotation vector $\boldsymbol{\theta}$, or a tensorial field such as the elastic distortion $\boldsymbol{\epsilon}^e$, the elastic rotation $\boldsymbol{\omega}^e$, or the elastic strain $\boldsymbol{\epsilon}^e$. We shall denote them either as *vectorial* or *tensorial* defect potentials, respectively.

2.2.1. *Vectorial defect potentials*

Consider the following four possible defect potentials in terms of the kinematic variable $\boldsymbol{\theta}$:

$$W^{(A1)}(\boldsymbol{\theta})=\frac{1}{2}\boldsymbol{\kappa}:\boldsymbol{\kappa},\ =\frac{1}{2}\boldsymbol{\kappa}:\mathbb{I}:\boldsymbol{\kappa}, \tag{38}$$

$$W^{(A2)}(\boldsymbol{\theta})=\frac{1}{2}\boldsymbol{\kappa}:\boldsymbol{\kappa}^T=\boldsymbol{\kappa}:\mathbb{I}^T:\boldsymbol{\kappa}, \tag{39}$$

$$W^{(A3)}(\boldsymbol{\theta}) = \frac{1}{2}\boldsymbol{\kappa} : \boldsymbol{\gamma} = \frac{1}{2}\boldsymbol{\kappa} : \mathbb{P} : \boldsymbol{\kappa} = \frac{1}{2}\boldsymbol{\gamma} : \mathbb{Q} : \boldsymbol{\gamma} \tag{40}$$

$$W^{(A4)}(\boldsymbol{\theta}) = \frac{1}{2}\boldsymbol{\kappa} : \boldsymbol{\gamma}^T = \frac{1}{2}\boldsymbol{\kappa} : \mathbb{S} : \boldsymbol{\kappa} = \frac{1}{2}\boldsymbol{\gamma} : \mathbb{T} : \boldsymbol{\gamma} \tag{41}$$

where $(\cdot)^T$ represents the transpose of $(\cdot)$. The dependence on $\boldsymbol{\theta}$ is based on the facts that $\boldsymbol{\kappa} = \nabla \times \boldsymbol{\theta}$ and $\boldsymbol{\gamma} = \mathbb{P} : \boldsymbol{\kappa}$. All four defect potentials in (38–41) quadratically depend on the curvature tensor $\boldsymbol{\kappa}$.

To check the variational character of the above defect potentials, we consider the following action functionals:

$$\Pi^{(Ai)}(\boldsymbol{\theta}) = \int_\Omega W^{(Ai)}(\boldsymbol{\theta}) \mathrm{d}\Omega, \quad i = 1, 2, 3, 4. \tag{42}$$

The Euler–Lagrange equations corresponding to the four potentials in (38–41) are given as follows:

$$\nabla \cdot \boldsymbol{\kappa} = 0, \quad \nabla \cdot \boldsymbol{\kappa}^T = 0, \quad \nabla \cdot \boldsymbol{\gamma} = 0, \quad \nabla \cdot \boldsymbol{\gamma}^T = 0. \tag{43}$$

To the best of the author's knowledge, among them, only the third Euler–Lagrange equation in (43), the one corresponding to the defect potential $W^{(A3)} = 1/2\ \boldsymbol{\gamma} : \boldsymbol{\kappa}$, is a meaningful balance law in physics, and its physical meaning is the manifestation of the conservation of the Burgers vector. In fact, by definition it reads exactly as

$$\nabla \cdot \boldsymbol{\gamma} = \nabla \cdot (\boldsymbol{\zeta} + \boldsymbol{\alpha}) = \nabla \cdot \boldsymbol{\alpha} = 0, \quad \Leftarrow \nabla \cdot \boldsymbol{\zeta} = \nabla \cdot \nabla \times \boldsymbol{\epsilon}^e \equiv 0. \tag{44}$$

Therefore we deem this defect potential as being variationally meaningful, because its Euler–Lagrange Equation (29) yields a valid *balance law* for the compatibility condition. This particular compatibility balance law or symmetry will be broken when there is a disclination distribution, see (35). For the other three defect potentials in (38), their validity as the variational potential are not clear to us at the moment, and it requires further study. Thus, in the rest of this paper, we shall only consider invariant properties of the defect potential

$$W^{(I)}(\boldsymbol{\theta}) := W^{(A3)}(\boldsymbol{\theta})$$

from this group of defect potentials. Again, we would like to point out that $W^{(I)}(\boldsymbol{\theta})$ is not convex in general.

2.2.2. *Tensorial defect potentials*

We now consider the defect potentials that can be expressed solely in terms of elastic distortion $\boldsymbol{\beta}^e$, elastic rotation $\boldsymbol{\omega}^e$, and elastic strain $\boldsymbol{\epsilon}^e$. So there are three groups of them.

(i) *Defect potentials in terms of elastic distortions* $\boldsymbol{\beta}^e$.
Consider the following four possible defect potentials in terms of elastic distortion $\boldsymbol{\beta}^e$:

$$W^{(B1)}(\boldsymbol{\beta}^e) = \frac{1}{2}\boldsymbol{\alpha} : \boldsymbol{\alpha} = \frac{1}{2}\boldsymbol{\alpha} : \mathbb{I} : \boldsymbol{\alpha}, \tag{45}$$

$$W^{(B2)}(\boldsymbol{\beta}^e) = \frac{1}{2}\boldsymbol{\alpha} : \boldsymbol{\alpha}^T = \frac{1}{2}\boldsymbol{\alpha} : \mathbb{I}^T : \boldsymbol{\alpha}, \tag{46}$$

$$W^{(B3)}(\boldsymbol{\beta}^e) = \frac{1}{2}\boldsymbol{\alpha} : \mathbf{K} = \frac{1}{2}\boldsymbol{\alpha} : \mathbb{Q} : \boldsymbol{\alpha} = \frac{1}{2}\mathbf{K} : \mathbb{P} : \mathbf{K} \tag{47}$$

$$W^{(B4)}(\boldsymbol{\beta}^e) = \frac{1}{2}\boldsymbol{\alpha} : \mathbf{K}^T = \frac{1}{2}\boldsymbol{\alpha} : \mathbb{T} : \boldsymbol{\alpha} = \frac{1}{2}\mathbf{K} : \mathbb{S} : \mathbf{K}. \tag{48}$$

The dependence on $\boldsymbol{\beta}^e$ occurs through the fact that $\boldsymbol{\alpha} = -\nabla \times \boldsymbol{\beta}^e$ and $\mathbf{K} = \mathbb{Q} : \boldsymbol{\alpha}$. All four defect potentials are quadratically dependent on the density of geometrically necessary dislocations, while only the first defect potentials in (45) is convex, and its Hessian tensor is positive definite. The first defect potential in (45) has been used as the elastic free energy in [28–32], among others. The third and the fourth defect potentials in (47) and (48) were first proposed by [11] as a Yang–Mills-type ansatz. Moreover, a related Euler–Lagragian equation has also been derived in [11]. Nonetheless, [11] attributed them to the Nye potentials, $(1/2)\boldsymbol{\alpha} : \boldsymbol{\kappa}^T$ and $(1/2)\boldsymbol{\alpha} : \boldsymbol{\kappa}$. [33] proposed a defect potential with a general form $(1/2)B_{ijk\ell}\alpha_{ij}\alpha_{k\ell}$. However, its variational character has not been studied.

To examine their variational characters, we consider the action functionals

$$\Pi^{(Bi)}(\boldsymbol{\beta}^e) = \int_\Omega W^{(Bi)}(\boldsymbol{\beta}^e)\mathrm{d}\Omega, \quad i = 1, 2, 3, 4. \tag{49}$$

Assume that the proper boundary conditions are prescribed. The Euler–Lagrange equations corresponding to the four potentials in (45–48) are as follows:

$$\nabla \times \boldsymbol{\alpha} = 0, \quad \nabla \times \boldsymbol{\alpha}^T = 0, \quad \nabla \times \mathbf{K} = 0, \quad \nabla \times \mathbf{K}^T = 0. \tag{50}$$

The first, the second, and the fourth Euler–Lagrange equation in (50) can be written in terms of the primary variable $\boldsymbol{\beta}^e$:

$$\delta\Pi^{(B1)} = 0 \Rightarrow \nabla \times \boldsymbol{\alpha} = 0 \rightarrow \nabla^2\boldsymbol{\beta}^e - \nabla \otimes (\nabla \cdot \boldsymbol{\beta}^e) = 0, \tag{51}$$

$$\delta\Pi^{(B2)} = 0 \Rightarrow \nabla \times \boldsymbol{\alpha}^T = 0 \rightarrow \nabla \times \boldsymbol{\beta}^e \times \nabla = 0, \tag{52}$$

$$\delta\Pi^{(B4)} = 0 \Rightarrow \nabla \times \mathbf{K}^T = 0 \rightarrow \nabla^2\boldsymbol{\beta}^e - \nabla \otimes (\nabla \cdot \boldsymbol{\beta}^e) = 0 \quad \text{and} \quad \nabla \times \boldsymbol{\beta}^e \times \nabla = 0. \tag{53}$$

All three equations will become identities, if there is no defect in a solid. However, we are not certain that they can serve as physical laws to characterize the compatibility condition in continuum. In other words, their variational characters are not very clear to us.

When there is no disclination in the solid,

$$\nabla \cdot \boldsymbol{\alpha} = 0, \Rightarrow \nabla \times \boldsymbol{\kappa} = \nabla \times \nabla \otimes \boldsymbol{\theta} \equiv 0, \tag{54}$$

one can show that

$$\nabla \times \mathbf{K} = \nabla \times \boldsymbol{\kappa} - \nabla \times \boldsymbol{\zeta}^T = \nabla \times \boldsymbol{\epsilon}^e \times \nabla. \tag{55}$$

Furthermore, if there are no dislocations or any other defects, the third equation in (50), $\delta\Pi^{(B3)} = 0 \Rightarrow \nabla \times \mathbf{K} = 0$, will reduce to the Saint-Venant compatibility equations.

Therefore, the third Euler–Lagrange equation is a meaningful physical law in its own right[1]. In fact, one can show that

$$\nabla \times \mathbf{K} = \nabla \times \boldsymbol{\epsilon}^e \times \nabla = -(\boldsymbol{\alpha} \times \nabla)_{\text{sym}} =: \mathfrak{Y} \tag{56}$$

where $\mathfrak{Y}$ is the so-called incompatibility tensor [22]. Thus we deem $W^{(B3)}(\boldsymbol{\beta})$ as variationally meaningful. We note that $W^{(B3)}$ may not always be convex and its Hessian tensor is not positive definite, because both $\mathbb{P}$ and $\mathbb{Q}$ are not positive definite. The convexity of $W^{(B3)}$ may depend on the actual dislocation distributions. In the rest of the paper, we only study the invariant properties of $W^{(II)}(\boldsymbol{\beta}^e) := W^{(B3)}(\boldsymbol{\beta}^e)$ among this group of defect potentials.

In [19], we take $W^{(B4)}$ as a primary *variational defect potential*. Whether or not that is a good choice and whether or not $W^{(B4)}$ is a variational defect potential remain to be seen. Moreover, we would like to point out that the defect potential $W^{(II)}(\boldsymbol{\beta}^e)$ is independent of the defect potential $W^{(I)}(\boldsymbol{\theta})$, and $W^{(II)}(\boldsymbol{\beta})$ is essentially a defect potential for dislocations while $W^{(I)}(\boldsymbol{\theta})$ is basically a defect potential for disclinations.

(ii) *Defect potentials in terms of elastic rotations* $\boldsymbol{\omega}^e$.
Next we consider the following group of tensorial defect potentials in terms of elastic rotations $\boldsymbol{\omega}^e$,

$$W^{(C1)}(\boldsymbol{\omega}^e) = \frac{1}{2}\boldsymbol{\gamma} : \boldsymbol{\gamma} = \frac{1}{2}\boldsymbol{\gamma} : \mathbb{I} : \boldsymbol{\gamma}, \tag{57}$$

$$W^{(C2)}(\boldsymbol{\omega}^e) = \frac{1}{2}\boldsymbol{\gamma} : \boldsymbol{\gamma}^T = \frac{1}{2}\boldsymbol{\gamma} : \mathbb{I}^T : \boldsymbol{\gamma}, \tag{58}$$

$$W^{(C3)}(\boldsymbol{\omega}^e) = \frac{1}{2}\boldsymbol{\gamma} : \boldsymbol{\kappa} = \frac{1}{2}\boldsymbol{\gamma} : \mathbb{Q} : \boldsymbol{\gamma} = \frac{1}{2}\boldsymbol{\kappa} : \mathbb{P} : \boldsymbol{\kappa}, \tag{59}$$

$$W^{(C4)}(\boldsymbol{\omega}^e) = \frac{1}{2}\boldsymbol{\gamma} : \boldsymbol{\kappa}^T = \frac{1}{2}\boldsymbol{\gamma} : \mathbb{T} : \boldsymbol{\gamma} = \frac{1}{2}\boldsymbol{\kappa} : \mathbb{S} : \boldsymbol{\kappa}. \tag{60}$$

All four defect potentials are dependent quadratically on either $\boldsymbol{\gamma}$ or $\boldsymbol{\kappa}$, which link to $\boldsymbol{\omega}^e$ through the fact that $\boldsymbol{\gamma} = -\nabla \times \boldsymbol{\omega}^e$ and $\boldsymbol{\kappa} = \mathbb{Q} : \boldsymbol{\gamma}$. Following the procedures used in the previous two group defect potentials, we can study their variational characters by examining the physical validity of the corresponding Euler–Lagrange equations.

One may find that the defect potentials $W^{(C3)}(\boldsymbol{\omega}^e)$ and $W^{(C4)}(\boldsymbol{\omega}^e)$ are identical to the defect potentials $W^{(A3)}(\boldsymbol{\theta})$ and $W^{(A4)}(\boldsymbol{\theta})$. So one may expect that they have the same invariant properties.

The Euler–Lagrange equations corresponding to the four potentials in (57–60) are given as

$$\nabla \times \boldsymbol{\gamma} = 0, \quad \nabla \times \boldsymbol{\gamma}^T = 0, \quad \nabla \times \boldsymbol{\kappa} = 0, \quad \nabla \times \boldsymbol{\kappa}^T = 0. \tag{61}$$

Both the first and second Euler–Lagrange equations in (61) are related to the compatibility condition of small rigid body rotation. In fact, the second Euler–Lagrange equation in (61) can be written as

$$\nabla \times \boldsymbol{\gamma}^T = 0 \rightarrow \nabla \times \boldsymbol{\omega}^e \times \nabla = 0, \tag{62}$$

resulting in compatibility equations in terms of elastic rotations $\boldsymbol{\omega}^e$. However, how to relate this condition to the integrability of strains is not clear to us. Similarly, we are not certain of the physical validity of the fourth equation.

As mentioned before, the third equation in (61) is an identity regardless of the presence of a continuous dislocation distribution, i.e.

$$\nabla \times \boldsymbol{\kappa} = \nabla \times \nabla \otimes \boldsymbol{\theta} \equiv 0. \tag{63}$$

Its physical meaning is the conservation of the Burgers vector. So $W^{(C3)}$ $(\boldsymbol{\omega}^e)$ is a variational defect potential, which is exactly the same as $W^{(A3)}$ $(\boldsymbol{\theta})$. The reason that the defect potential of (40) is identical to the defect potential of (59) is because of the relationship between the rotation vector $\boldsymbol{\theta}$ and the elastic rotation $\boldsymbol{\omega}^e$ given in (12). No matter which of the two potentials is used in deriving conservation laws, the result will be the same, since they are both describing the defect state measured by local elastic rotation of the continuum. Therefore, we shall not treat it as an independent case in the study of variational symmetry. We note, however, both (40) and (59) are essentially disclination defect potentials, and Equation (63) is no longer held when there is disclination distribution. Therefore, to be absolutely certain that the two defect potentials are identical, it may depend on the choice of disclination theory adopted in calculations. For now, we denote $W^{(Ib)} := W^{(C3)}(\boldsymbol{\omega}^e)$ as an alternative of $W^{(I)} := W^{(A3)}(\boldsymbol{\theta})$.

(iii) *Defect potentials in terms of the elastic strain* $\boldsymbol{\epsilon}^e$.
Finally, we consider the following two defect potentials in terms of the curl of the elastic strain $\boldsymbol{\zeta}$,

$$W^{(D1)}(\boldsymbol{\epsilon}^e) = \frac{1}{2}\boldsymbol{\zeta} : \boldsymbol{\zeta} = \frac{1}{2}\boldsymbol{\zeta} : \mathbb{I} : \boldsymbol{\zeta} \tag{64}$$

$$W^{(D2)}(\boldsymbol{\epsilon}^e) = \frac{1}{2}\boldsymbol{\zeta} : \boldsymbol{\zeta}^T = \frac{1}{2}\boldsymbol{\zeta} : \mathbb{I}^T : \boldsymbol{\zeta}. \tag{65}$$

The dependence on $\boldsymbol{\epsilon}^e$ stems from of the fact that $\boldsymbol{\zeta} = \nabla \times \boldsymbol{\epsilon}^e$.

The Euler–Lagrange equations corresponding to the two potentials in (64) and (65) can be obtained by considering the stationary condition

$$\delta\Pi^{(Di)} = \delta \int_\Omega W^{(Di)}(\boldsymbol{\epsilon}^e)\mathrm{d}\Omega = 0, \quad i = 1, 2$$

which leads to

$$\nabla \times \boldsymbol{\zeta} = 0 \quad \text{and} \quad \nabla \times \boldsymbol{\zeta}^T = 0. \tag{66}$$

$W^{(D1)}(\boldsymbol{\epsilon}^e)$ is always convex. However, its Euler–Lagrange Equations (66) are not strain compatibility conditions, even though they become identities when there is no defect in the solid. For the time being, we cannot identify their physical meanings.

The second set of Euler–Lagrange equations in (66), which correspond to the defect potential $W^{(D2)}(\boldsymbol{\epsilon}^e)$, was first derived in [34] via a so-called Saint-Venant variational principle. This can be written as

$$\nabla \times \boldsymbol{\zeta}^T = 0 \rightarrow \nabla \times \boldsymbol{\epsilon}^e \times \nabla = 0, \tag{67}$$

resulting in the Saint-Venant compatibility equations in terms of the elastic strains $\boldsymbol{\epsilon}^e$. Therefore, between the defect potentials, $W^{(D1)}(\boldsymbol{\epsilon}^e)$ and $W^{(D2)}(\boldsymbol{\epsilon}^e)$, we deem $W^{(III)}(\boldsymbol{\epsilon}^e) := W^{(D2)}(\boldsymbol{\epsilon}^e)$ as variationally meaningful.

3. Compatibility conservation laws

In this section, we study the variational symmetry of defect potentials chosen in the last section. Once the potential functionals are chosen, the derivation of conservation laws is a straightforward application of Noether's theorem [1,20,35]. Depending on the nature of the primary variable of the chosen variational defect potential, meaning that whether its argument is vectorial or tensorial, different versions of Noether's theorems are applied. We proceed by first listing all three variational defect potentials

$$W^{(I)}(\boldsymbol{\theta}) = \frac{1}{2}\boldsymbol{\gamma} : \mathbb{Q} : \boldsymbol{\gamma}, \quad W^{(II)}(\boldsymbol{\beta}^e) = \frac{1}{2}\boldsymbol{\alpha} : \mathbb{Q} : \boldsymbol{\alpha}, \quad \text{and} \quad W^{(III)} = \frac{1}{2}\boldsymbol{\zeta} : \mathbb{I}^T : \boldsymbol{\zeta}. \tag{68}$$

The Euler–Lagrange equations corresponding to the following potential functionals,

$$\Pi^{(i)} = \int_\Omega W^{(i)}(\boldsymbol{\theta}) \mathrm{d}\Omega, \quad i = I, II, III \tag{69}$$

are

$$(I) \nabla \cdot \boldsymbol{\gamma} = 0, \quad (II) \nabla \times \mathbf{K} = 0, \quad \text{and} \quad (III) \nabla \times \boldsymbol{\epsilon}^e \times \nabla = 0. \tag{70}$$

Applying Noether's theorem to the potential functionals (69), we obtain the following three classes of compatibility conservation laws (**CL-1**)–(**CL-3**),

$$(I) \begin{cases} S^{(I)}_{k\alpha} = W^{(I)}\delta_{k\alpha} - \theta_{\ell,\alpha}\gamma_{k\ell} & \rightarrow \quad L^{(I)}_\alpha = \oint_S S^{(I)}_{k\alpha} n_k \mathrm{d}S \\ T^{(I)}_{k\alpha} = e_{\alpha\ell\beta}\left(x_\ell S^{(I)}_{k\beta} + \theta_\ell \gamma_{k\beta}\right) & \rightarrow \quad F^{(I)}_\alpha = \oint_S T^{(I)}_{k\alpha} n_k \mathrm{d}S \\ U^{(I)}_k = x_\alpha S^{(I)}_{k\alpha} - \frac{1}{2}\theta_\ell \gamma_{k\ell} & \rightarrow \quad G^{(I)} = \oint_S U^{(I)}_k n_k \mathrm{d}S \\ P^{(I)}_{k\alpha} = \gamma_{k\alpha} & \rightarrow \quad H^{(I)}_\alpha = \oint_S P^{(I)}_{k\alpha} n_k \mathrm{d}S \end{cases} \tag{71}$$

$$(II) \begin{cases} S^{(II)}_{k\alpha} = W^{(II)}\delta_{k\alpha} - e_{kmi}K_{mj}\beta^e_{ij,\alpha} & \rightarrow \quad L^{(II)}_\alpha = \oint_S S^{(II)}_{k\alpha} n_k \mathrm{d}S \\ T^{(II)}_{k\alpha} = e_{j\beta\alpha}\left(x_j S^{(II)}_{k\beta} + e_{pki}K_{pj}\beta^e_{i\beta}\right) & \\ \qquad +\delta_{k\alpha}K_{mj}\beta^e_{mj} - K_{\alpha j}\beta^e_{kj} & \rightarrow \quad F^{(II)}_\alpha = \oint_S T^{(II)}_{k\alpha} n_k \mathrm{d}S \\ U^{(II)}_k = W^{(II)}x_k + \frac{1}{2}e_{mki}K_{mj}\left(\beta^e_{ij} + 2\beta^e_{ij,\ell}x_\ell\right) & \rightarrow \quad G^{(II)} = \oint_S U^{(II)}_k n_k \mathrm{d}S \\ P^{(II)}_k = -e_{mki}K_{mj}f_{ij} & \rightarrow \quad H^{(II)} = \oint_S P^{(II)}_k n_k \mathrm{d}S \end{cases}$$

$$(III)\begin{cases} S^{(III)}_{k\alpha} = W^{(III)}\delta_{k\alpha} - e_{mki}\zeta_{mj}\epsilon^{e}_{ij,\alpha} & \rightarrow \quad L^{(III)}_{\alpha} = \oint_S S^{(III)}_{k\alpha} n_k \mathrm{d}S \\ T^{(III)}_{k\alpha} = e_{j\beta\alpha}\left(x_j S^{(III)}_{k\beta} + e_{mki}\zeta_{\beta m}\epsilon^{e}_{ij}\right) & \\ \qquad -\delta_{k\alpha}\zeta_{j\beta}\epsilon^{e}_{\beta j} + \zeta_{j\alpha}\epsilon^{e}_{kj} & \rightarrow \quad F^{(III)}_{\alpha} = \oint_S T^{(III)}_{k\alpha} n_k \mathrm{d}S \\ U^{(III)}_{k} = W^{(III)}x_k - \dfrac{1}{2}e_{mki}\zeta_{mj}\left(\epsilon^{e}_{ij} + 2\epsilon^{e}_{ij,\ell}x_\ell\right) & \rightarrow \quad G^{(III)} = \oint_S U^{(III)}_{k} n_k \mathrm{d}S \\ P^{(III)}_{k} = e_{mki}\zeta_{jm}c_{ij} & \rightarrow \quad H^{(III)} = \oint_S P^{(III)}_{k} n_k \mathrm{d}S. \end{cases}$$

Since $\boldsymbol{\epsilon}^{e} \in Sym$, we have two more conservation laws as follows:

$$\begin{cases} P^{(III)}_{k\alpha} = e_{mk\alpha}\zeta_{mj}c_j + e_{mki}\zeta_{m\alpha}c_i & \rightarrow \quad H^{(III)}_{\alpha} = \oint_S P^{(III)}_{k\alpha} n_k \mathrm{d}S \\ P^{(III)}_{ijk} = e_{mki}\zeta_{mj} & \rightarrow \quad H^{(III)}_{ij} = \oint_S P^{(III)}_{ijk} n_k \mathrm{d}S. \end{cases} \tag{72}$$

The first class of conservation laws (**CL-1**) has the following equivalent class (**CL-1b**):

$$(Ib)\begin{cases} S^{(Ib)}_{k\alpha} = W^{(Ib)}\delta_{k\alpha} - e_{kmi}\kappa_{mj}\omega^{e}_{ij,\alpha} & \rightarrow \quad L^{(Ib)}_{\alpha} = \oint_S S^{(Ib)}_{k\alpha} n_k \mathrm{d}S \\ T^{(Ib)}_{k\alpha} = e_{j\beta\alpha}\left(x_j S^{(Ib)}_{k\beta} + e_{pki}\kappa_{pj}\omega^{e}_{i\beta}\right) & \\ \quad +\delta_{k\alpha}\kappa_{mj}\omega^{e}_{mj} - \kappa_{\alpha j}\omega^{e}_{kj} & \rightarrow \quad F^{(Ib)}_{\alpha} = \oint_S T^{(Ib)}_{k\alpha} n_k \mathrm{d}S \\ U^{(Ib)}_{k} = W^{(Ib)}x_k + \dfrac{1}{2}e_{mki}\kappa_{mj}\left(\omega^{e}_{ij} + 2\omega^{e}_{ij,\ell}x_\ell\right) & \rightarrow \quad G^{(Ib)} = \oint_S U^{(Ib)}_{k} n_k \mathrm{d}S \\ P^{(Ib)}_{k} = -e_{mki}\kappa_{mj}f_{ij} & \rightarrow \quad H^{(Ib)} = \oint_S P^{(Ib)}_{k} n_k \mathrm{d}S. \end{cases} \tag{73}$$

For all three (four) variational defect potentials selected, none of them are convex, therefore they may not be suitable as the exact elastic free energy expression for stable materials in a continuum thermodynamics theory. However, they may serve as part of the free-energy measure in defect zones.

The physical meaning of the derived quantity, $S^{(i)}_{k\alpha}$, $i = I, II, III$, is the change of the defect potentials $W^{(i)}$, $i = I, II, III$ when a defect moves. In an analogy to Eshelby's energy–momentum tensor, we denote the new quantity as the *compatibility–momentum tensor*. The origin of the variational defect potential discussed in this paper is different from or independent of the dislocation free-energy, and they stem from kinematic or geometric compatibility conditions rather than energetic conditions, though the variational defect potentials may be used to measure or calibrate the dislocation core energy. Indeed, in the dislocation gauge theory, several constitutive relations have been postulated by using similar potentials to construct a total elastic free-energy expression, e.g. [11,36,37] among others. We label this approach as the *free-energy formulation*

approach or the *free-energy formalism*. In fact, one reason to do so is to seek a 'generalized free-energy expression' that reflects the compatibility condition, e.g. [38,39]. This, in the author's opinion, is beyond the original notion of the configurational force in the sense of Eshelby, which is completely based on energetic conditions at the thermodynamics equilibrium state, though it might be included in the sense of Gurtin, which is based on irreversible continuum thermodynamics arguments. Moreover, many dislocation free-energies proposed in the literature may *not* be variationally meaningful, that is: the Euler–Lagrange equations derived from the corresponding potential functional may not be a physical law or an established geometric relation, e.g. [27,32]. Moreover, most of the proposed free-energy potentials are convex, and their Hessian matrices are positive definite in order to satisfy thermodynamics constraints. On the other hand, we are not certain that the non-convex variational defect potentials discussed here can be used as legitimate candidates for the strain gradient free-energy of stable materials. Thus the conservation laws discussed here mainly provide integrability conditions for defect motions, which are, in principle, not related to the configurational force derived from energetic conditions at the equilibrium state. We shall discuss this issue again in later sections.

It is noted that the related contour integrals of compatibility conservation laws (71) are path-independent, even if there is a dislocation distribution, or as long as the Burgers vector is conserved. This type of conservation law breaks down when there is a disclination distribution. If the kinematic defect potential is rescaled to a proper energetic quantity, a configurational force stemming from this type of conservation law may serve as the material force acting on the disclination.

Remark 3.1: It is true that in linear elasticity the Saint-Venant compatibility conditions can be obtained as the Euler–Lagrange equation of the minimum complementary potential energy principle, e.g. [40]. This is often done in terms of the stress function formulation. Because it is often believed that the complementary energy–momentum tensor of the complementary potential energy is different from that of strain energy potential, e.g. [41,42], the present author has studied the variational symmetry of the two-dimensional complementary potential energy in terms of the Airy stress function ([43]).

However, the stress function approach has several limitations. First, it is only valid for linear elastic materials, whereas the compatibility conservation laws derived in this paper are much more general and independent of the constitutive relations, and hence they can be applied to any material. In fact, the objective of this paper is to develop invariant integrals for inelastic media to measure the energy release rate due to defect motions or distributions. Second, the stress function approach is not directly related to kinematic variables such as strains, distortions, etc. and it is often difficult to convert the stress function to kinematic variables due to different orders of derivatives.

4. A multiscale Griffith criterion

It has become a consensus now that macroscopically brittle fracture is a multiscale phenomenon. The first milestone of fracture mechanics is A.A. Griffith's energy criterion for brittle crack growth [44], which has been extensively used in solving elastic fracture mechanics (LEFM) problems. For ductile fracture, the matter is more complex, and the Griffith criterion may not be applicable. By recognizing that ductile fracture is a multiscale

problem, Irwin [45] proposed the Griffith–Irwin criterion for ductile crack growth under the condition of small-scale yielding. Even though Irwin's criterion has been illustrated convincingly through physical arguments, it has never been justified in rigorous mathematical analysis. In this section, we shall use one of the compatibility–momentum tensors derived in the previous sections to study macroscopically brittle fracture under small-scale yielding conditions.

To distinguish the different scales, we decompose the displacement field of a deformed solid into a coarse-scale field and a fine-scale field:

$$\mathbf{u}(\mathbf{x}) = \bar{\mathbf{u}}(\mathbf{x}) + \mathbf{u}'(\mathbf{x}) \tag{74}$$

where $\bar{\mathbf{u}}$ is the coarse (macro)scale displacement field, which may be viewed as a homogenized field, and $\mathbf{u}'$ is the fine (micro)scale displacement field, which may be affected by the fluctuation of defect distributions or micro-structures. Moreover, we assume that the fine-scale defect distribution is localized – the very assumption of the small-scale yielding condition–so that a global homogenization will still yield a linear elastic coarse-scale deformation field. The total strain field can thus decompose to

$$\boldsymbol{\beta} = \bar{\boldsymbol{\beta}} + \boldsymbol{\beta}' = \bar{\boldsymbol{\beta}} + \boldsymbol{\beta}^{e\prime} + \boldsymbol{\beta}^{p\prime} = \boldsymbol{\beta}^{e} + \boldsymbol{\beta}^{p} \tag{75}$$

where $\bar{\boldsymbol{\beta}} = \bar{\boldsymbol{\beta}}^{e} = \nabla \otimes \bar{\mathbf{u}}$, and both $\boldsymbol{\beta}'_{e}$ and $\boldsymbol{\beta}'_{p}$ are incompatible elastic and plastic strains. Note that $\boldsymbol{\beta}^{e} = \bar{\boldsymbol{\beta}}^{e} + \boldsymbol{\beta}^{e\prime}$ and $\boldsymbol{\beta}^{p} = \boldsymbol{\beta}^{p\prime}$. We now define a *multiscale free-energy measure*,

$$W^{m}(\bar{\mathbf{u}}, \boldsymbol{\epsilon}^{e\prime}) = W^{c}(\bar{\mathbf{u}}) + W^{f}(\boldsymbol{\beta}^{e\prime}) \tag{76}$$

where the coarse-scale strain energy density is

$$W^{c} = \frac{1}{2}\bar{\boldsymbol{\epsilon}}^{e} : \bar{\mathbb{C}} : \bar{\boldsymbol{\epsilon}}^{e} \tag{77}$$

and $\bar{\mathbb{C}}$ is the coarse-scale elastic stiffness tensor. The fine-scale *free-energy measure* is constructed as

$$W^{f}(\boldsymbol{\beta}^{e\prime}) := \mu\ell^{2} W^{(II)}(\boldsymbol{\beta}^{e\prime}) = \frac{\mu\ell^{2}}{2}\boldsymbol{\alpha} : \mathbf{K} = \frac{\mu\ell^{2}}{2}\boldsymbol{\alpha} : \mathbb{Q} : \boldsymbol{\alpha} \tag{78}$$

where μ is the elastic shear modulus, and ℓ is a length-scale, below which the coarse-scale observer cannot see. Note that the scaling factor, $\mu\ell^{2}$, makes the unit of the re-scaled $W^{(II)}$ up to strain energy density. Since $\boldsymbol{\alpha} = -\nabla \times \boldsymbol{\beta}^{e} = -\nabla \times \boldsymbol{\beta}^{e'}$, one can choose either of them as the state variable. Note that $\boldsymbol{\alpha} : \mathbb{Q} : \boldsymbol{\alpha} \not> 0$, though it is convex for the special anti-plane problem that will be discussed next. We note that there are major differences between the *multiscale free energy measure approach* proposed here and the *free energy formulation approach* commonly used in strain gradient theories, e.g. [26,46,47] as well as in the dislocation gauge theory, e.g. [76]:

(1) In the multiscale theory, $\boldsymbol{\epsilon}^{e'}(\mathbf{x})$ is not related to any displacement gradient, and (76) suggests a mixed variational principle. Under the small-scale yielding assumption (Irwin's argument), the fine-scale defect distribution or fluctuation is highly localized, so it won't affect the macroscale constitutive relation. In other words, the coarse-scale displacement field $\bar{\mathbf{u}}(\mathbf{x})$ is decoupled from the fine-scale strain field, $\boldsymbol{\epsilon}^{e'}(\mathbf{x})$. One may also argue that because a given macroscale displacement field can

correspond to many microscale strain fields, in mathematics, the inverse of a given homogenized field is never unique. Therefore, the coarse-scale fields and the fine-scale fields are virtually independent. Consequently, one can decouple $W^c(\bar{\mathbf{u}})$ and $W^f(\boldsymbol{\epsilon}^{e\prime})$ in multiscale theory; whereas in the strain gradient theory or the dislocation gauge theory, the two free-energy terms are always coupled, either through equilibrium equation or constitutive relations. Hence the macroscale elastic strain free-energy will always affect, or be affected by, the microscale constitutive relations.

(2) The multiscale *free energy measure* is not a free energy expression or a free energy per se, it is rather a *free energy measurement or calibration*. The fine-scale free energy measure standard is given a priori, no matter what the actual microscale constitutive relations are and no matter where the actual fine-scale free energy comes from. We can only use the fine-scale *free-energy measure*, which may be an approximation of an essential part of fine-scale free-energy, to extrapolate existing elastic free energy information from given defect distributions. However it is not enough nor is it intended to determine the fine-scale constitutive relation. In the multiscale approach, the fine-scale *free-energy measure* is a universal entity, which is independent of the actual constitutive make-up, whereas in the strain gradient theory or the dislocation gauge theory one usually has a higher-order (fine-scale) free-energy first, and then one uses it to derive the constitutive relations at the fine scale, and eventually one would hope to use them solving for defect distributions as well as defect motions. Only until after that is done, one can come back again to calculate the configurational force at the equilibrium state, provided that the problem is still tractable. In short, the free-energy formalism approach determines both macro- and microscale constitutive relations, whereas the multiscale free-energy measure approach proposed in this work only provides a universal measure to calibrate the existing free energy stored in a solid, which is actually independent of the microscale constitutive relations.

(3) Another distinguishing feature of the fine-scale *free-energy measure approach* proposed in this work is that its defect potentials are non-convex, therefore their stationary points may not be related to the attainment of an equilibrium state, and it is possible that they are related to the attainment of a metastable state. Thus, the subsequent configurational force derived based on the present approach may be considered as a generalization to the classical Eshelbian configurational force of thermodynamical equilibrium states.

To illustrate the validity of the free-energy calibration approach, we assume that: (1) $\bar{\boldsymbol{\sigma}} := \partial W^c / \partial \bar{\boldsymbol{\epsilon}}^e$ where $\bar{\boldsymbol{\sigma}}$ is the coarse-scale Cauchy stress, and (2) there is an a priori defect distribution represented by the incompatibility tensor

$$\mathfrak{Y} := -\mathrm{inc}(\boldsymbol{\epsilon}^p) = -\nabla \times \boldsymbol{\epsilon}^p \times \nabla, \quad \text{and} \quad \mathfrak{T} := \frac{\mu \ell^2}{2}(\mathbb{I} + \mathbb{I}^T) : \mathfrak{Y} \tag{79}$$

where $\mathfrak{T}$ is the related internal stress. Consider the following multiscale elastic potential with the prescribed deformation condition,

$$\Pi^m = \int_\Omega \left(W^m(\bar{\mathbf{u}}, \boldsymbol{\beta}^{e\prime}) - \mathbf{f} \cdot \bar{\mathbf{u}} - \mathfrak{T} : \boldsymbol{\beta}^{e\prime} \right) \mathrm{d}\Omega, \quad \text{with } \delta\bar{\mathbf{u}} = 0 \quad \text{and} \quad \delta\boldsymbol{\beta}^{e\prime} = 0, \quad \forall \mathbf{x} \in \partial\Omega. \tag{80}$$

One may find that

$$\delta\Pi^m = \int_\Omega \Big(\frac{\partial W^c}{\partial \bar{\boldsymbol{\epsilon}}^e} : \delta\bar{\boldsymbol{\epsilon}}^e + \frac{\partial W^f}{\partial \boldsymbol{\alpha}} : \delta\boldsymbol{\alpha} - \mathbf{f}\cdot\delta\bar{\mathbf{u}} - \mathfrak{T} : \delta\boldsymbol{\beta}^{e\prime} \Big) \mathrm{d}\Omega$$
$$= -\int_\Omega \Big\{ \Big(\nabla\cdot\bar{\boldsymbol{\sigma}} + \mathbf{f} \Big)\cdot\delta\bar{\mathbf{u}} + \Big(\mu\ell^2 \mathrm{inc}(\boldsymbol{\epsilon}^{e\prime}) - \mathfrak{T} \Big) : \delta\boldsymbol{\beta}^{e\prime} \Big\} \mathrm{d}\Omega \tag{81}$$

which leads to a set of universal multiscale field equations

$$\nabla\cdot\bar{\boldsymbol{\sigma}} + \mathbf{f} = 0, \quad \text{and} \quad \mu\ell^2 \mathrm{inc}(\boldsymbol{\epsilon}^{e\prime}) = \mathfrak{T}, \quad \forall \mathbf{x} \in \Omega. \tag{82}$$

Obviously, the detailed fine-scale constitutive relations do not come into play, except that we use the fine-scale shear modulus μ in the construction of multiscale free energy measure.

Based on Noether's theorem, the coordinate translation invariance leads to the following multiscale energy–momentum tensor

$$\mathcal{S}_{k\alpha} = S^c_{k\alpha} + S^f_{k\alpha} \tag{83}$$

where $S^c_{k\alpha}$, $S^f_{k\alpha}$ are the coarse and fine scale energy-momentum tensors with superscripted indicators, respectively. The coarse-scale energy momentum tensor $S^c_{k\alpha}$ is the Eshelby energy momentum tensor [4,5] for the background elastic medium,

$$S^c_{k\alpha} = W^c\delta_{k\alpha} - u_{\ell,\alpha}\sigma_{k\ell} \tag{84}$$

where u_ℓ are the total displacements of the elastic fields, and $\sigma_{k\ell}$ are the Cauchy stress components. Note that the subscript, $(\,)_{,i}$, denotes the spatial derivatives.

The fine-scale energy–momentum tensor is obtained as the scaled compatibility tensor $S^2_{k\alpha}$ (see Table 2),

$$S^f_{k\alpha} = W^f\delta_{k\alpha} - \mu\ell^2 e_{kmi}K_{mj}\beta^e_{ij,\alpha}. \tag{85}$$

We can then obtain a *multiscale configurational force*,

$$\mathcal{L}_\alpha = J_\alpha + L_\alpha \tag{86}$$

where the coarse-scale configurational force is the J-integral [48] for the linear elastic solid,

$$\bar{J}_\alpha := \oint_S S^c_{k\alpha} n_k \mathrm{d}S$$

Table 2. List of compatibility–momentum tensors, $S^{(i)}_{k\alpha}$, $i = I, Ib, II, III$.

$W^{(i)}$, $i = I, Ib, II, III$	E-L equations	$S^{(i)}_{k\alpha}, i = I, Ib, II, III$
$W^{(I)} = (1/2)\boldsymbol{\kappa} : \boldsymbol{\gamma}$	$\nabla\cdot\boldsymbol{\gamma}0$	$W^{(I)}\delta_{k\alpha} - \theta_{\ell,\alpha}\gamma_{k\ell}$
$W^{(Ib)} = (1/2)\boldsymbol{\kappa} : \boldsymbol{\gamma}$	$\nabla\times\boldsymbol{\kappa} = 0$	$W^{(Ib)}\delta_{k\alpha} - e_{kmi}\kappa_{mj}\omega^e_{ij,\alpha}$
$W^{(II)} = (1/2)\boldsymbol{\alpha} : \mathbf{K}$	$\nabla\times\mathbf{K} = 0$	$W^{(II)}\delta_{k\alpha} - e_{kmi}K_{mj}\beta^e_{ij,\alpha}$
$W^{(III)}) = (1/2)\boldsymbol{\zeta} : \boldsymbol{\zeta}^T$	$\nabla\times\boldsymbol{\zeta}^T = 0$	$W^{(III)}\delta_{k\alpha} - e_{kmi}\zeta_{jm}\epsilon^e_{ij,\alpha}$

and the fine-scale configurational force is the re-scaled L-integral,

$$L_\alpha := \oint_S S^f_{k\alpha} n_k \mathrm{d}S \tag{87}$$

Table 3. Field quantities in the elastic region Ω_e and the plastic region Ω_p.

Field	Elastic region Ω_e	Plastic region Ω_p
$\boldsymbol{\sigma}$	$\frac{K_{III}}{\sqrt{2\pi r}}\begin{bmatrix} 0 & 0 & -\sin\frac{\theta}{2} \\ 0 & 0 & \cos\frac{\theta}{2} \\ -\sin\frac{\theta}{2} & \cos\frac{\theta}{2} & 0 \end{bmatrix}$	$\tau_0\begin{bmatrix} 0 & 0 & -\sin\frac{\theta}{2} \\ 0 & 0 & \cos\frac{\theta}{2} \\ -\sin\frac{\theta}{2} & \cos\frac{\theta}{2} & 0 \end{bmatrix}$
$\boldsymbol{\epsilon}^e$	$\frac{K_{III}}{2\mu\sqrt{2\pi r}}\begin{bmatrix} 0 & 0 & -\sin\frac{\theta}{2} \\ 0 & 0 & \cos\frac{\theta}{2} \\ -\sin\frac{\theta}{2} & \cos\frac{\theta}{2} & 0 \end{bmatrix}$	$\frac{\tau_0}{2\mu}\begin{bmatrix} 0 & 0 & -\sin\frac{\theta}{2} \\ 0 & 0 & \cos\frac{\theta}{2} \\ -\sin\frac{\theta}{2} & \cos\frac{\theta}{2} & 0 \end{bmatrix}$
$\boldsymbol{\beta}^e$	$\frac{K_{III}}{\mu\sqrt{2\pi r}}\begin{bmatrix} 0 & 0 & -\sin\frac{\theta}{2} \\ 0 & 0 & \cos\frac{\theta}{2} \\ 0 & 0 & 0 \end{bmatrix}$	$\frac{\tau_0}{\mu}\begin{bmatrix} 0 & 0 & -\sin\frac{\theta}{2} \\ 0 & 0 & \cos\frac{\theta}{2} \\ 0 & 0 & 0 \end{bmatrix}$

Table 4. Defect densities in the elastic region Ω_e and the plastic region Ω_p.

Field	$\forall \mathbf{x} \in \Omega_e$	$\forall \mathbf{x} \in \Omega_p$
$\boldsymbol{\alpha}$	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	$-\frac{\tau_0}{2r\mu}\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \cos\frac{\theta}{2} \end{bmatrix}$
$\boldsymbol{\gamma}$	$-\frac{K_{III}}{4r\mu\sqrt{2\pi r}}\begin{bmatrix} \cos\frac{3\theta}{2} & \sin\frac{3\theta}{2} & 0 \\ \sin\frac{3\theta}{2} & -\cos\frac{3\theta}{2} & 0 \\ 0 & 0 & 0 \end{bmatrix}$	$-\frac{\tau_0}{4r\mu}\begin{bmatrix} \cos\frac{\theta}{2}\cos\theta & \sin\frac{\theta}{2}\cos\theta & 0 \\ \cos\frac{\theta}{2}\sin\theta & \sin\frac{\theta}{2}\sin\theta & 0 \\ 0 & 0 & \cos\frac{\theta}{2} \end{bmatrix}$
$\boldsymbol{\zeta}$	$-\frac{K_{III}}{4r\mu\sqrt{2\pi r}}\begin{bmatrix} \cos\frac{3\theta}{2} & \sin\frac{3\theta}{2} & 0 \\ \sin\frac{3\theta}{2} & -\cos\frac{3\theta}{2} & 0 \\ 0 & 0 & 0 \end{bmatrix}$	$-\frac{\tau_0}{4r\mu}\begin{bmatrix} \cos\frac{\theta}{2}\cos\theta & \sin\frac{\theta}{2}\cos\theta & 0 \\ \cos\frac{\theta}{2}\sin\theta & \sin\frac{\theta}{2}\sin\theta & 0 \\ 0 & 0 & -\cos\frac{\theta}{2} \end{bmatrix}$

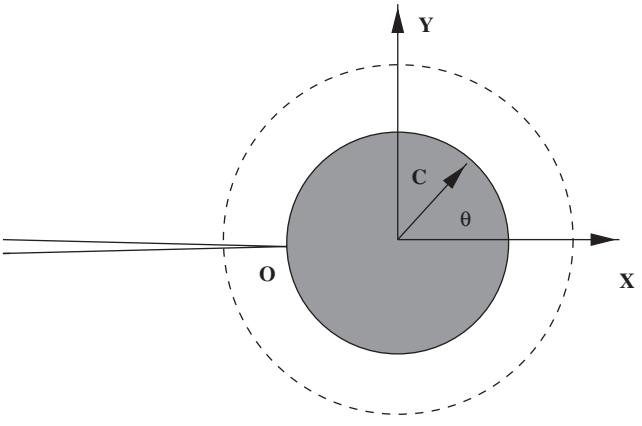

Figure 1. Schematic illustration of a macroscopically brittle crack.

which can be used to measure the elastic free-energy stored inside the plastic zone in front of an elasto-plastic crack of small-scale yielding. Because both integrals are path-independent, their linear combination should also be path-independent, if the solid is defect-free. In the rest of this paper, we denote the first component of $\mathcal{L}_\alpha$ as the multiscale L-integral, i.e. $L^m = \mathcal{L}_1$, which may represent the driving force for a macroscopically brittle crack.

For simplicity, we consider a self-similar and steady state crack growth solution of mode-III crack (see Figure 1) in a linearly elastic and perfectly plastic solid, whose solution is available ([49]). As a benchmark solution, we view the Hult–McClintock (HM) solution as a reasonably good approximation of such multiscale problems. For easy reference, we document the HM solution in terms of defect measures in Tables 3 and 4.

We now calculate L^m–integral for the mode-III steady state solution of the elasto-plastic crack (the Hult–McClintock solution). The integration contour is taken as the boundary of plastic zone, S. The coarse-scale J-integral is taken over on a slightly larger contour, $\Gamma_c = S^+$, than the plastic zone in order to include the crack tip. The fine-scale L_1 integral path is over a slightly smaller contour, $\Gamma_f = S^-$ (see Figure 2). Suppose the crack length is denoted as a, and the remote stress is τ_∞. The multiscale driving force is

$$L^m = \left(\frac{\pi\tau_\infty^2}{2\mu}\right)a + \left(\frac{3\mu\ell^2\pi\tau_0^2}{16\mu c}\right) \tag{88}$$

in which the radius of the plastic zone, c, can be related to the crack length a by $c = a\tau_\infty^2/2\tau_0^2$ and hence

$$L^m = \left(\frac{\pi\tau_\infty^2}{2\mu}\right)a + \left(\frac{3\ell^2\pi\tau_0^4}{8\mu\tau_\infty^2}\right)\frac{1}{a}. \tag{89}$$

A fundamental task of fracture mechanics is to determine the critical stress, $\tau_{\rm cr}$, under which the crack advances. Based on the Griffith criterion, the critical stress is obtained by setting the equilibrium condition, i.e. the driving force equals the resistance force. We now

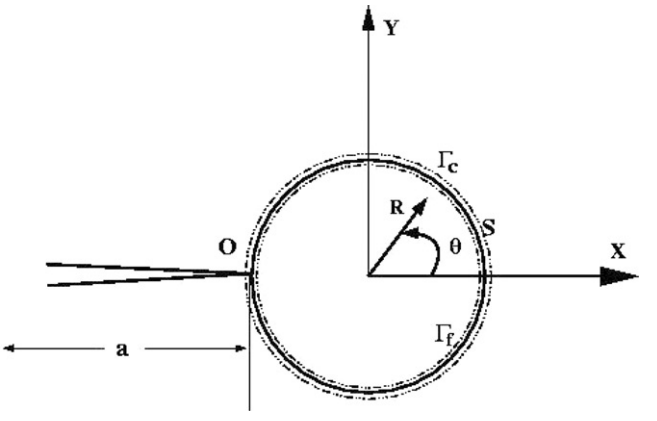

Figure 2. Schematic illustration of the contour path of the multiscale invariant integrals.

invoke Griffith's energetic argument [44] and equate the multiscale driving force to the resistance:

$$L^m = \left(\frac{\pi a}{2\mu}\right)(\tau_{\rm cr})^2 + \left(\frac{3\ell^2\pi\tau_0^4}{8\mu a}\right)\frac{1}{(\tau_{\rm cr})^2} = 2\gamma_t. \tag{90}$$

We observe that the multiscale driving force has two parts: (1) the coarse-scale part, i.e. the release of elastic strain energy, or the value of the J-integral in a purely elastic medium,

$$J = \frac{\pi a(\tau_{\rm cr})^2}{2\mu},$$

and (2) the fine-scale part due to the release of the elastic free-energy stored inside a dislocation distribution zone, or plastic zone,

$$\tilde{L} = \left(\frac{3\ell^2\pi\tau_0^4}{8\mu a\tau_{\rm cr}^2}\right).$$

Note that in the multiscale Griffith equation the first part of the driving force may no longer be equal to the resistance due to surface separation, i.e. $2\gamma_s$. In other words, the strain energy release due to the reduction of elastic potential in the elastic region will not be solely consumed in the surface separation. To expedite the analysis, we introduce a critical length-scale, $\ell_{\rm cr} := 4/\sqrt{3}(\gamma_t\mu/\pi\tau_0^2)$, which may depend on the resistance.

We scale the energy release with a reference resistance energy, $2\gamma_0 := \pi\ell{\tau_0}^2/2\mu$, which may be viewed as the fracture resistance that the theoretical strength of the material can offer for an ideally brittle crack. Then, the ratio

$$I(\ell) := \frac{J}{2\gamma_0} = \frac{\pi a(\tau_{\rm cr})^2/2\mu}{\pi\ell\tau_0^2/2\mu} = \left(\frac{a}{\ell}\right)\left(\frac{\tau_{\rm cr}(a)}{\tau_0}\right)^2 \tag{91}$$

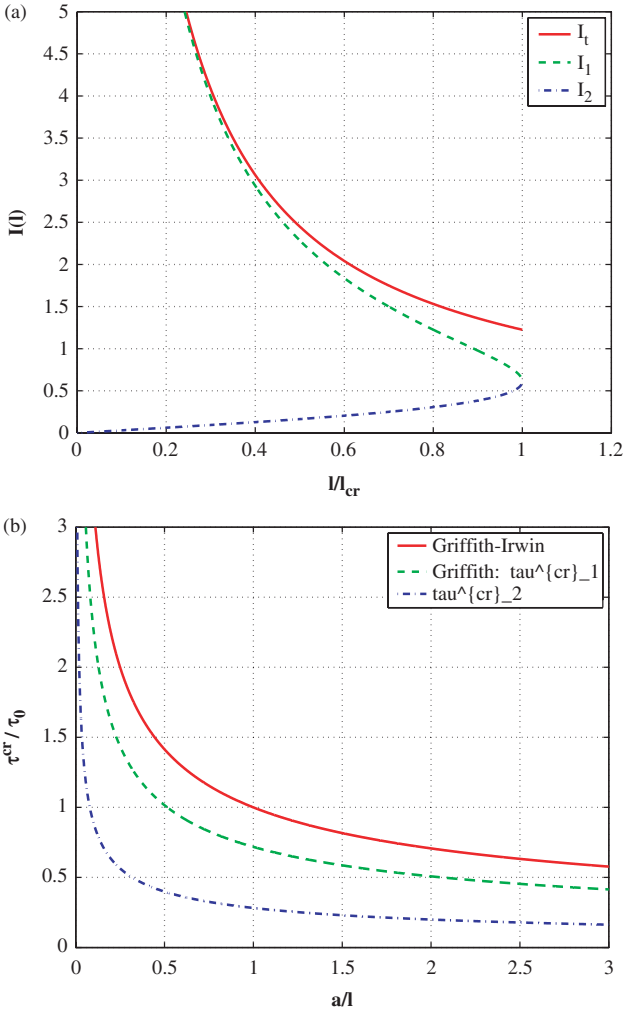

Figure 3. (a) Bifurcated solutions $I_i(\ell)$, $i=1,2$ vs. $\ell/\ell_{\rm cr}$; and (b) the critical stresses vs. a/ℓ: (1) Griffith–Irwin stress $\tau_I^{\rm cr}/\tau_0$, (2) multiscale solution $\tau_1^{\rm cr}/\tau_0$, and (3) multiscale solution $\tau_2^{\rm cr}/\tau_0$.

is a function of the length-scale ℓ. The symbol I is in honor of G.R. Irwin. Subsequently, the multiscale Griffith Equation (90) is normalized as

$$I(\ell)+\frac{3}{4}\frac{1}{I(\ell)}=\frac{4\gamma_t\mu}{\pi\ell\tau_0^2}=\sqrt{3}\left(\frac{\ell_{\rm cr}}{\ell}\right). \tag{92}$$

Unlike the classical Griffith equation, the multiscale Griffith Equation (92) is a quadratic equation in terms of $I(\ell)$; it yields two solutions:

$$I(\ell)_{1,2}=\frac{I_t(\ell)}{2}\left[1\pm\sqrt{1-\left(\frac{\ell}{\ell_{\rm cr}}\right)^2}\right]=\left(\frac{\gamma_t}{2\gamma_0}\right)\left[1\pm\sqrt{1-(\frac{\ell}{\ell_{\rm cr}})^2}\right] \tag{93}$$

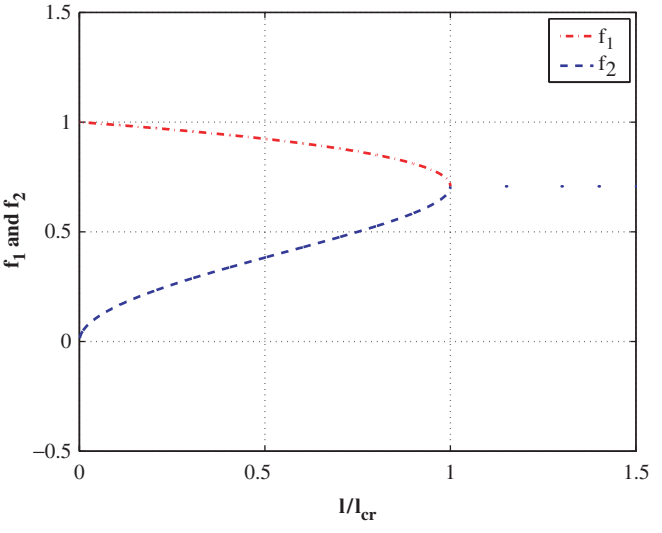

Figure 4. Scaling factors of energy release rates.

where $I_t(\ell)$ is the normalized total resistance at the equilibrium,

$$I_t(\ell) = \gamma_t/\gamma_0 = \sqrt{3}\left(\frac{\ell_{\rm cr}}{\ell}\right). \tag{94}$$

To compare the different energy release rates, we plot the two normalized $I_i(\ell)$, $i=1,2$ and I_t in Figure 3(a). One may find that the two solutions of I_i bifurcate at $\ell=\ell_{cr}$. The total energy release rate or the resistance at equilibrium, I_t, is the sum of the two.

Using the definition (91), we find the corresponding critical stresses as follows:

$$\tau^{\rm cr}_{1,2} = \tau_0\sqrt{\frac{\ell I_{1,2}(\ell)}{a}} = \sqrt{\frac{4\mu\gamma_t}{a\pi}}\left[\frac{1}{2}\left(1 \pm \sqrt{1-\left(\frac{\ell}{\ell_{\rm cr}}\right)^2}\right)\right]^{1/2} = \tau^{\rm cr}_I f(\ell)_{1,2} \tag{95}$$

where

$$\tau^{\rm cr}_I := \sqrt{\frac{4\mu\gamma_t}{a\pi}} \tag{96}$$

denotes the critical Griffith–Irwin stress, and the two scaling factors are defined as

$$f_{1,2}(\ell) := \left[\frac{1}{2}\left(1 \pm \sqrt{1-\left(\frac{\ell}{\ell_{\rm cr}}\right)^2}\right)\right]^{1/2}, \tag{97}$$

which are plotted in Figure 4. To fully understand the meanings of these two solutions of energy release rate, we calculated the asymptotic expression for the critical stresses $\tau_1^{\rm cr}$, and $\tau_2^{\rm cr}$,

$$\tau_1^{\rm cr} = \tau_0\sqrt{\frac{I_1(\ell)}{a/\ell}} \approx \sqrt{\frac{4\gamma_t\mu}{\pi a}} + \mathcal{O}(\ell), \quad \text{and} \quad \tau_2^{\rm cr} = \tau_0\sqrt{\frac{I_2(\ell)}{a/\ell}} \approx \tau_0\sqrt{\frac{3\pi\ell^2\tau_0^2}{16a\gamma_t\mu}} + \mathcal{O}(\ell). \tag{98}$$

One can find that the stress corresponding to $I_1(\ell)$ is independent of the yield stress, τ_0. This indicates that the first solution, $I_1(\ell)$, may be related to the resistance to the surface separation, i.e. $I_1(\ell) \sim \gamma_s/\gamma_0$, where γ_s is the resistance due to surface separation. On the other hand, one may find in (98)(b) that τ_2 depends on the yield stress τ_0, and hence we identify that $I_2(\ell)$ corresponds to the normalized resistance due to incompatible defect fields, or the dislocation field. That is $I_2(\ell) \sim \gamma_p/\gamma_0$, where γ_p denotes the energy dissipation due to the incompatible field evolution.

Fortuitously, the two roots of the multiscale Griffith Equation (93) have an interesting property,

$$I_1(\ell) + I_2(\ell) = I_t(\ell) = \frac{\gamma_t}{\gamma_0}. \tag{99}$$

At equilibrium I_1 and I_2 can be interpreted as resistances, and based on the above arguments, we know that I_1 and I_2 link to different types of resistances. This suggests that we can express the total fracture resistance as an addictive superposition of two distinct sources.

$$\gamma_t = \gamma_s + \gamma_p.$$

This conclusion is not trivial because the problem under consideration is nonlinear (the HM solution is a nonlinear solution). It then leads to a modified critical stress expression:

$$\tau_I^{\rm cr} = \sqrt{\frac{4\mu(\gamma_s + \gamma_p)}{\pi a}}$$

which is the essential result of Irwin's multiscale theory of elasto-plastic fracture under small-scale yielding (see Figure 3(b)). In the multiscale analysis $\tau_I^{\rm cr} \geq \tau_1^{\rm cr}, \tau_2^{\rm cr}$. Thus, it is natural to choose $\tau_I^{\rm cr}$ as the critical stress, because it captures the overall effects of both I_1 and I_2. To the best knowledge of the author, this is the first rigorous justification of Irwin's theory [45] by using multiscale analysis and the continuum theory of dislocations.

A summary of the results presented here has been reported early in a letter [50]. However, in ([50]), we choose $W^f = \mathrm{W}^{(III)}(\boldsymbol{\epsilon}^e)$, though the numerical results of the two approaches are identical. This confirms our early speculation that $W^{(II)}(\boldsymbol{\beta}^e)$ is equivalent to $W^{(III)}(\boldsymbol{\epsilon}^e)$.

5. Closure

In this paper, we have studied the invariant theory of continuum dislocations and its application to fracture. We presented a variational defect potential theory and derived three classes of compatibility conservation laws and the corresponding invariant integrals.

In contrast to the conservation laws of classical continuum mechanics, which are based on equilibrium conditions, the derived conservation law was based on compatibility conditions, therefore they can be valid at a much smaller length-scale. We would like to point out again that by no means have we exhausted all the possibilities of compatibility conservation laws in continuum mechanics. By utilizing such conservation laws, we first formed a multiscale configurational force, and then we proposed a multiscale Griffith criterion for elasto-plastic fracture under small-scale yielding. The proposed multiscale formulation rigorously justifies the well-known Griffith-Irwin theory. We note that the multiscale Griffith criterion proposed in this paper has its own limitation too. It may only be valid at sub-micron length-scales where the strain gradient effect is most significant. Any scale effects below that scale cannot be captured by the present theory. An extension of the present theoretical framework to solids under finite deformation will be reported in subsequent work.

Acknowledgements

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Note

1. See the comments made in [22], pp. 245–246.

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