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On configurational compatibility and multiscale energy momentum tensors

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Abstract

In this work the continuum theory of defects has been revised through the development of kinematic defect potentials. These defect potentials and their corresponding variational principles provide a basis for constructing a new class of conservation laws associated with the compatibility conditions of continua. These conservation laws represent configurational compatibility conditions which are independent of the constitutive behavior of the continuum. They lead to the development of a new concept termed configurational compatibility, dual to the concept of configurational force. The contour integral of the corresponding conserved quantity is path-independent, if the domain encompassed by the integral is defect-free. It is shown that the Peach–Koehler force can be recovered as one of these invariant integrals. Based on the proposed defect potentials and their corresponding defect energies, two-field multiscale mixed variational principles can be employed to construct multiscale energy momentum tensors. An application is outlined in the form of a mode III elasto-plastic crack problem for which the new configurational quantities are calculated.

Keywords: Conservation integrals; Dislocations; Fracture; Multiscale analysis; Strain compatibility

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1. Introduction

Fracture of materials is one of the most studied problems in material science and applied mechanics. The first milestone of *fracture mechanics* is Griffith's seminal work (Griffith, 1921) on the fracture of glass rods. Griffith postulated that crack propagation occurs when the potential energy release resulting from an increment of crack growth is sufficient to overcome the surface energy of the material. In the Griffith model, the fracture resistance is assumed to come exclusively from the surface energy of the material and restricts the application to brittle materials. Irwin (1948) extended Griffith's approach to metals by including the energy dissipated by local plastic flow. These concepts served as the basis of classical *linear elastic fracture mechanics*. The foundation of the modern theory for crack extension is due to the landmark contributions of Eshelby (1951, 1956) and Rice (1968). In the quasi-static case, one may show that the *J*-integral is equivalent to the energy release rate for an elastic body. For inelastic materials, the situation becomes more complex. In metallic systems, the stress concentration at the crack tip may enable dislocation emission. One of the first models to examine brittle (cleavage) and ductile (dislocation emission) behavior was formulated by Rice and Thomson (1974). A more refined theory of dislocation nucleation based on the Peierls–Nabarro model (Peierls, 1940; Nabarro, 1952) was later proposed by Rice (1992). Subsequent experimental findings (Jokl et al., 1989; Huang and Gerberich, 1992; Zielinski et al., 1992; Marsh et al., 1992; George and Michot, 1993) and recent results of large scale atomistic simulations (Grujicic and Du, 1995; Cleri et al., 1997; Zhou et al., 1997; Bulatov et al., 1998; Cleri et al., 1998; Farkas, 1998; Waghmare et al., 2000; Farkas, 2000; Farkas et al., 2001; Bernstein and Hess, 2003; Guo et al., 2003; Mattoni et al., 2005; Farkas, 2005) have suggested that the fracture of brittle materials is a multiscale phenomenon involving cleavage, dislocation emission, and a host of grain and grain boundary dependent mechanisms such as twinning, recrystallization, or phase transformation. Today, it has become a general consensus that fracture is an archetype of multiscale phenomena in condensed solid state physics.

In addition to experimental and computational findings, another focus of contemporary fracture mechanics is the study of *configurational mechanics*. Motivated by the belief that the configurational structure of the material is intrinsic to defect mechanics, configurational mechanics has become a framework for modelling defects. Continuum descriptions in material space contrast the Newtonian approach to mechanics in physical space. Literature on this topic can be found in Maugin (1993), Gurtin (1999), Kienzler and Herrmann (2000), Kienzler and Maugin (2002), and Steinmann and Maugin (2005), among others. Well-known examples of configurational forces on defects are the Peach–Koehler force (Peach and Koehler, 1950) and the *J*-integral (Eshelby, 1951, 1956; Rice, 1968).

The objective of the current work is to explore the relationship between the motion of defects and configurational mechanics. The concept of configurational forces is based on conservation laws in elasticity which are a manifestation of the symmetry properties of equilibrium equations. Recently, in an effort to search for kinematic conservation laws of elasticity, symmetry properties of kinematic conditions of the continuum have been studied in Li (2004), Li et al. (2005) and Li and Gupta (2006). Based on the duality between forces (equilibrium) and kinematics (compatibility) in continuum mechanics, it is natural to argue that such a duality also exists in the framework of configurational mechanics. This leads to the proposal of a concept termed *configurational compatibility*, dual to the well-established notion of *configurational force*. Our approach to configurational compatibility is through the construction of a defect potential based on the continuum theory of dislocations. One of the early proposals for a dislocation theory was brought forward by Burgers (1939) which included an expression for the displacement field of a dislocation loop in terms of line integrals over its length and an area integral over its enclosed area. Peach and Koehler (1950) derived an expression for the configurational force on a dislocation segment. Nye's curvature tensor (Nye, 1953) has been found to be a useful equivalent of the dislocation density which is a measure of defects inside the continuum. Kondo (1952) and Bilby et al. (1955) independently developed a dislocation theory in the context of differential geometry. Kröner (1958, 1960) and Kröner and Seeger (1959) extended this theory to a non-linear theory of elasticity with dislocations and internal stress. Mura (1968) and Willis (1970) transformed Burgers' equation into a line integral for displacement gradients in terms of an integrand containing the elastic Green function tensor. The incorporation of disclinations was achieved by Anthony (1970) and deWit (1970) among others. More recent contributions in this active field can be found in Kröner (1981), Teodosiu (1982), Davini (1986), Naghdi and Srinivasa (1994), Steinmann (1996), Arsenlis and Parks (1999), Davini (2001), Kröner (2001), Parry (2001), Cermelli and Gurtin (2001), Gurtin (2002). The short list cited here is far from being complete.

From the viewpoint of multiscale modelling, the stress defined in continuum mechanics is a macroscale quantity, which originates from the homogenization or idealization of a continuum ensemble. Therefore, the configurational force derived from the equilibrium of such stresses should also be considered a macroscale quantity. No configurational force based on a microscale stress, such as the virial stress (Clausius, 1870; Lutsko, 1988; Cormier et al., 2001; Zhou, 2003) or Hardy's stress (Hardy, 1982; Zimmerman et al., 2004), has been reported. In contrast, the incompatibility of the lattice is a concept of microscale or even of atomic scale if the solid has a well-defined lattice structure. This suggests that compatibility conservation laws may be able to capture the physics of the microscale. Compared to the classical conservation laws based on stress equilibrium conditions, conservation laws stemming from configurational compatibility will be valid at a much smaller length scale. Therefore, it is natural to institute the concept of multiscale configurational mechanics by combining the conservation laws based on equilibrium, valid at the coarse scale (macroscale), with those based on compatibility, valid at the fine scale (microscale). Combining coarse scale and fine scale energy densities yields the second concept in this work, the *multiscale energy momentum tensor*. It will be shown that the multiscale energy momentum tensor is composed of a coarse scale component, Eshelby's energy momentum tensor (Eshelby, 1951) and a fine scale component, a scaled compatibility momentum tensor. The constructed multiscale framework will be applied to mode III crack propagation. Ramifications of the new framework include a multiscale driving force.

The paper is organized in six sections. We start in Section 2 by revising the linear continuum theory of dislocations through the construction of defect potentials. In Section 3, we introduce the concept of configurational compatibility and present a new class of kinematic conservation laws based on the proposed defect potential. In Section 4, multiscale energy momentum tensors are derived from coarse scale and fine scale potentials. Configurational compatibility and multiscale energy momentum tensors are applied to a mode III elasto-plastic crack problem in Section 5. We close the presentation in Section 6 by making a few concluding remarks.

2. Defect potentials based on the linear continuum theory of dislocations

In this section we will review the main aspects of the well-established *linear continuum theory of dislocations* and propose defect potentials subsequently used to construct the concepts of configurational compatibility and multiscale energy momentum tensors.

To fix the notation, we first introduce the convention used to describe dislocations, outline the assumptions made in deriving the theory, and then focus on the construction of a valid defect potential. We identify a perfectly ordered state as a defect-free state. Crystals are commonly classified as the most ordered structures of mass points. In order to obtain a continuum description of the crystal, a limiting process is performed. If the crystal is not defect-free, we obtain a continuum description of the defect. Identifying dislocations as the main defect in this work, we obtain a continuum theory of dislocations. The incorporation of plasticity into the continuum was achieved by decomposing the total strain ε_{ij} of the plastic solid into an elastic part $\varepsilon^{\mathrm{e}}_{ij}$, which gives rise to stresses based on the general assumptions of elasticity theory, and a plastic or inelastic part $\varepsilon^{\mathrm{p}}_{ij}$, which changes the shape of the solid and leads to permanent deformation. In the infinitesimal case, this decomposition is given as

$$\varepsilon_{ij} = \varepsilon^{\mathrm{e}}_{ij} + \varepsilon^{\mathrm{p}}_{ij}. \tag{1}$$

Contrary to ε_{ij}, which is always a compatible field, $\varepsilon^{\mathrm{e}}_{ij}$ and $\varepsilon^{\mathrm{p}}_{ij}$ are, in general, not compatible fields. Since the plastic deformation is permanent, the elastic strain $\varepsilon^{\mathrm{e}}_{ij}$ no longer satisfies the compatibility equations, which will be affected by a defect distribution that constitutes inelastic deformations. The continuum defect theory is formulated with elastic or inelastic kinematic variables in order to represent the defect distribution. Even though the elastic strain $\varepsilon^{\mathrm{e}}_{ij}$ is a state quantity, which means that it can be uniquely measured at any time, it is not enough to describe the influence of dislocations in the body (Kröner, 1958). The curvature, which serves as another state quantity, plays a dominant role in the continuum theory of defects, as it will be shown below. Following Kröner (1958, 1960, 1981), we introduce the corresponding anti-symmetric rotation tensors ω_{ij}, ω^{e}_{ij}, ω^{p}_{ij}, and distortion tensors β_{ij}, β^{e}_{ij}, β^{p}_{ij} as

$$\beta_{ij} = \varepsilon_{ij} + \omega_{ij}, \quad \beta^{\mathrm{e}}_{ij} = \varepsilon^{\mathrm{e}}_{ij} + \omega^{\mathrm{e}}_{ij} \quad \text{and} \quad \beta^{\mathrm{p}}_{ij} = \varepsilon^{\mathrm{p}}_{ij} + \omega^{\mathrm{p}}_{ij}, \tag{2}$$

with the analogous decomposition as (1), namely

$$\omega_{ij} = \omega^{\mathrm{e}}_{ij} + \omega^{\mathrm{p}}_{ij} \quad \text{and} \quad \beta_{ij} = \beta^{\mathrm{e}}_{ij} + \beta^{\mathrm{p}}_{ij}. \tag{3}$$

In order to describe how points in the body are transferred by the total distortion β_{ij}, we introduce the total displacement vector as

$$\mathrm{d}u_j = \beta_{ij}\,\mathrm{d}x_i. \tag{4}$$

The term distortion is used instead of displacement gradient, because the β's are gradients as in (4) only if the corresponding deformation is compatible. This is the case for the total distortion but in general does no longer hold for the elastic and plastic distortion. Based on the total displacement vector u_j we can write the total distortion β_{ij}, the total strains ε_{ij} and the total rotations ω_{ij} as

$$\beta_{ij} = u_{j,i}, \quad \varepsilon_{ij} = \tfrac{1}{2}(u_{j,i} + u_{i,j}) \quad \text{and} \quad \omega_{ij} = \tfrac{1}{2}(u_{j,i} - u_{i,j}). \tag{5}$$

In order to describe the defect, which is mainly referred as the dislocation in this work, we define the *geometrically necessary dislocation density* according to Kröner (1958, 1960, 1981) in terms of the plastic distortion tensor

$$\alpha_{ij} := e_{ik\ell}\beta^{\mathrm{p}}_{\ell j,k}, \tag{6}$$

where the permutation symbol $e_{ik\ell}$ has been used. Since the total distortion $\beta_{\ell j}$ has to remain compatible, namely $e_{ik\ell}\beta_{\ell j,k} = 0$ has to be satisfied which means that the body is not allowed to break, we can rewrite (6) as

$$\alpha_{ij} = -e_{ik\ell}\beta^{\mathrm{e}}_{\ell j,k}. \tag{7}$$

The condition of the conservation of Burgers' vector follows directly from (7) as

$$\alpha_{ij,i} = 0, \tag{8}$$

which implies that dislocations do not end inside the body. The physical interpretation of (8) is the conservation of net Burgers' vector since

$$\oint_S \alpha_{ij} n_i \,\mathrm{d}S = b_j. \tag{9}$$

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

$$\omega^{\mathrm{e}}_{ij} = e_{ijk}\theta_k \quad \text{or} \quad \theta_k = \tfrac{1}{2} e_{ijk}\omega^{\mathrm{e}}_{ij}, \tag{10}$$

where θ_k is the axial vector of the elastic rotation ω^{e}_{ij}. Based on (10), we can further write

$$e_{ik\ell}\omega^{\mathrm{e}}_{\ell j,k} = e_{ik\ell}e_{\ell jm}\theta_{m,k} = \theta_{k,k}\delta_{ij} - \theta_{i,j}, \tag{11}$$

where the Kronecker symbol δ_{ij} has been used. Now we can use (2), (7), and (11) to obtain the following expression for the geometrically necessary dislocation density

$$\alpha_{ij} = -e_{ik\ell}\varepsilon^{\mathrm{e}}_{\ell j,k} + \theta_{i,j} - \theta_{k,k}\delta_{ij}. \tag{12}$$

If we introduce the curvature κ_{ij} as $\kappa_{ij} := \theta_{j,i}$, we can rewrite (12) as

$$\alpha_{ij} = -e_{ik\ell}\varepsilon^{\mathrm{e}}_{\ell j,k} + \kappa_{ji} - \kappa_{kk}\delta_{ij}. \tag{13}$$

Taking into account that $e_{ik\ell}\varepsilon^{\mathrm{e}}_{\ell i,k} = 0$ allows us, based on (13), to compute the trace of the curvature κ_{kk} in terms of the trace of the geometric necessary dislocation density α_{kk} as $\kappa_{kk} = -\frac{1}{2}\alpha_{kk}$, which further allows us to write the inverse relation of (13) as

$$\kappa_{ij} = e_{jk\ell}\varepsilon^{\mathrm{e}}_{\ell i,k} + \alpha_{ji} - \tfrac{1}{2}\alpha_{kk}\delta_{ij}. \tag{14}$$

Summarizing (13) and (14), we have the following kinematic relations,

$$\begin{aligned} \alpha_{ij} &= -e_{ik\ell}\varepsilon^{\mathrm{e}}_{\ell j,k} + \kappa_{ji} - \kappa_{kk}\delta_{ij}, \\ \kappa_{ij} &= e_{jk\ell}\varepsilon^{\mathrm{e}}_{\ell i,k} + \alpha_{ji} - \tfrac{1}{2}\alpha_{kk}\delta_{ij}. \end{aligned} \tag{15}$$

Eqs. (15), which are extensively used in the open literature, are the basic formulas in the continuum theory of dislocations. One way to simplify (15) is to neglect the contribution from the elastic strain gradients, by assuming $e_{ik\ell}\varepsilon^{\mathrm{e}}_{\ell j,k} = 0$ as in Kröner (1958, 1960, 1981), which results in

$$\begin{aligned} \alpha_{ij} &= \kappa_{ji} - \kappa_{kk}\delta_{ij}, \\ \kappa_{ij} &= \alpha_{ji} - \tfrac{1}{2}\alpha_{kk}\delta_{ij}. \end{aligned} \tag{16}$$

Eq. (15) can also be simplified by introducing the contortion K_{ij} (deWit, 1970) as

$$K_{ij} := \kappa_{ij} - e_{jk\ell}\varepsilon^{e}_{\ell i,k}. \tag{17}$$

The contortion K_{ij} is a measure of incompatibility and considered to be a source quantity rather than a field quantity like the curvature κ_{ij} (deWit, 1970). Since $K_{ii} = \kappa_{ii}$, (15) can be written as

$$\alpha_{ij} = K_{ji} - K_{kk}\delta_{ij},$$
$$K_{ij} = \alpha_{ji} - \tfrac{1}{2}\alpha_{kk}\delta_{ij}. \tag{18}$$

One approach proposed by Nye (1953) is to use a "dislocation potential" to study a geometrical object. Stimulated by Nye's dislocation potential in kinematics (Nye, 1953), we will construct a defect potential in terms of the dislocation density α_{ij} and the contortion K_{ij} in the form

$$W = \tfrac{1}{2}\alpha_{ij}K_{ji}. \tag{19}$$

Remark 1. The proposed defect potential (19) in terms of the geometrically necessary dislocation density α_{ij} and the transpose of the contortion K_{ij} should not be confused with existing dislocation potentials in terms of the geometrically dislocation density α_{ij} and the curvature κ_{ij} as in Nye (1953), where originally a defect potential in the form $\frac{1}{2}\alpha_{ij}\kappa_{ij}$ has been used. A quadratic form of the geometrically necessary dislocation density α_{ij} as $\frac{1}{2}\alpha_{ij}\alpha_{ij}$ is often used to incorporate the defect contribution to the free energy (Steinmann, 1996; Kröner, 2001; Gurtin, 2002; Clayton et al., 2004). There may exist other defect potentials (Li et al., 2006) which may provide further insight to the physical understanding of defects in solids.

In the next section, (19) is used as the departure point for the construction of configurational compatibility within the infinitesimal theory. A single defect potential is presented to clearly illustrate the methodology, even though other defect potentials may yield similar results (Li et al., 2006).

3. Configurational compatibility

Based on the defect potential in (19), in this section we will construct conservation laws stemming from kinematic relations for the infinitesimal theory. This procedure is instrumental in leading to the discovery of *configurational compatibility*, a concept dual to the concept of *configurational force*. We proceed by adopting the standard variational approach, which is based on Noether's theorem (Noether, 1918), though other approaches (Gurtin, 1995) may be possible.

To motivate our approach, we first recall that when applying Noether's theorem (Noether, 1918; Logan, 1977; Olver, 1986; Ibragimov, 1994; Li et al., 2005, 2006) to the potential energy (Knowles and Sternberg, 1972)

$$\Pi^{(1)}(\mathbf{u}) := \int_{\Omega} W^{(1)}(\nabla\mathbf{u})\,\mathrm{d}\Omega \quad \text{where } W^{(1)} := \frac{1}{2}\sigma_{ij}\varepsilon_{ij}, \tag{20}$$

of an elastic body, where no decomposition (1) or (3) is required, whose Euler–Lagrange equations can be written in terms of the elasticity tensor $C_{ijk\ell}$ as

$$C_{ijk\ell}u_{\ell,ki} = 0 \quad \forall\mathbf{x}\in\Omega \quad \text{and} \quad u_i = \bar{u}_i \quad \forall\mathbf{x}\in\partial\Omega, \tag{21}$$

under coordinate translation with ε_{ij} and σ_{ij} as the strains and stresses, respectively, results in the conserved quantity

$$E_{k\alpha} = W^{(1)}\delta_{k\alpha} - u_{\ell,\alpha}\sigma_{k\ell} \tag{22}$$

which is Eshelby's energy momentum tensor (Eshelby, 1951). If body forces are absent, we can write $\sigma_{k\alpha,k} = 0$. For this case, one can easily verify that $E_{k\alpha}$ is divergence-free, which can be expressed as $E_{k\alpha,k} = 0$. This leads to the invariant integrals

$$J_\alpha = \oint_S E_{k\alpha} n_k \,\mathrm{d}S, \tag{23}$$

which are zero, provided that there are no defects inside the integral contour. For $\alpha = 1$, we obtain the J-integral (Rice, 1968) which represents the configurational force acting on a defect.

Contrary to these well-known developments of configurational forces and conservation laws based on the equilibrium equations (21), we will focus in the remaining part of this section on the compatibility equations of a body. Following the same procedure as above for deriving the conservation laws based on the equilibrium equations, we will now derive a new class of compatibility conservation laws. The stresses σ_{ij}, introduced in (20), will only reappear in Remark 5, a possible application of the derived compatibility conservation laws.

In the following we will first state the variational principle and its corresponding Euler–Lagrange equations. Then, we will apply Noether's theorem for chosen symmetry groups to the Lagrangian and derive the corresponding class of compatibility conservation laws and their corresponding path-independent integrals.

3.1. The variational principle and corresponding Euler– Lagrange equations

In order to construct conservation laws stemming from kinematic relations, we will use defect potential (19) in terms of the dislocation density α_{ij} and the contortion K_{ij} as

$$W^{(2)} := \tfrac{1}{2}\alpha_{ij}K_{ji}, \tag{24}$$

with $\alpha_{ij} = -e_{ik\ell}\beta^{\mathrm{e}}_{\ell j,k}$ and $K_{ij} = \alpha_{ji} - \frac{1}{2}\alpha_{kk}\delta_{ij}$ given in (7) and (18), respectively. We assume that the elastic distortion β^{e}_{ij} is prescribed on $\partial\Omega$. Then the stationary condition $\delta_{\beta^{\mathrm{e}}}\Pi^{(2)} = 0$ of the following fundamental integral

$$\Pi^{(2)}(\boldsymbol{\beta}^{\mathrm{e}}) := \int_\Omega W^{(2)}(\boldsymbol{\beta}^{\mathrm{e}}_{,i})\,\mathrm{d}\Omega, \tag{25}$$

results in the Euler–Lagrange equations

$$-e_{ik\ell}K_{j\ell,k} = 0 \quad \forall \mathbf{x} \in \Omega \quad \text{and} \quad \beta^{\mathrm{e}}_{ij} = \bar{\beta}^{\mathrm{e}}_{ij} \quad \forall \mathbf{x} \in \partial\Omega, \tag{26}$$

stating that the curl of the transpose of the contortion vanishes inside Ω.

Remark 2. (a) Note that the Euler–Lagrange equation (26) $\forall \mathbf{x} \in \Omega$ can alternatively be written in terms of the elastic distortion as $\beta^{\mathrm{e}}_{\ell j,kk} - \beta^{\mathrm{e}}_{kj,\ell k} = 0$ together with $e_{ik\ell}e_{jmn}\beta^{\mathrm{e}}_{nj,mk} = 0$.

(b) Based on Remark 1, the Euler–Lagrange equations corresponding to the defect potential $\frac{1}{2}\alpha_{ij}\kappa_{ij}$ used in Nye (1953) are given as $\nabla \times \boldsymbol{\beta}^{\mathrm{e}} \times \nabla = \mathbf{0}$ and $e_{ik\ell}e_{jmn}\beta^{\mathrm{e}}_{nj,mk} = 0$, where the second equation corresponds to the second Euler–Lagrange equation in

Remark 2(a). For the quadratic defect potential $\frac{1}{2}\alpha_{ij}\alpha_{ij}$ the Euler–Lagrange equation is given as $\beta^{\mathrm{e}}_{\ell j,kk} - \beta^{\mathrm{e}}_{kj,\ell k} = 0$, which corresponds to the first Euler–Lagrange equation in Remark 2(a). We conclude that $\frac{1}{2}\alpha_{ij}\alpha_{ij}$ is a special case of $W^{(2)}$.

3.2. The compatibility conservation laws

Based on the Lagrangian (26), we will derive the corresponding conservation laws (**CL**) and path-independent integrals in this section.

Theorem 3. *Consider a simply connected continuum under infinitesimal deformation. Let* $\Omega \in \mathbb{R}^3$ *with Lipschitz continuous boundary* $\partial\Omega$. *Assume that the elastic distortion* $\beta^{\mathrm{e}}_{ij}(\mathbf{x})$ *satisfies the tensorial differential equations given in* (26). *Based on the result of Noether's theorem for a tensorial field* (Li et al., 2006), *the following compatibility conservation laws hold together with their path-independent integrals*:

$$\textbf{CL1}.\ S_{k\alpha} = W^{(2)}\delta_{k\alpha} - e_{kmi}K_{jm}\beta^{\mathrm{e}}_{ij,\alpha} \to L_\alpha = \oint_S S_{k\alpha}n_k\,\mathrm{d}S, \tag{27}$$

$$\begin{aligned}\textbf{CL2}.\ T_{k\alpha} &= W^{(2)}e_{jk\alpha}x_j + e_{pki}K_{jp}(e_{m\ell\alpha}x_m\beta^{\mathrm{e}}_{ij,\ell} - e_{mj\alpha}\beta^{\mathrm{e}}_{im}) + \delta_{k\alpha}K_{jm}\beta^{\mathrm{e}}_{mj} - K_{j\alpha}\beta^{\mathrm{e}}_{kj}\\ &\to F_\alpha = \oint_S T_{k\alpha}n_k\,\mathrm{d}S,\end{aligned} \tag{28}$$

$$\textbf{CL3}.\ U_k = W^{(2)}x_k + \frac{1}{2}e_{mki}K_{jm}(\beta^{\mathrm{e}}_{ij} + 2\beta^{\mathrm{e}}_{ij,\ell}x_\ell) \to G = \oint_S U_k n_k\,\mathrm{d}S, \tag{29}$$

$$\textbf{CL4}.\ P_k = -e_{mki}K_{jm}f_{ij} \to H = \oint_S P_k n_k\,\mathrm{d}S, \tag{30}$$

where $W^{(2)} = \frac{1}{2}\alpha_{ij}K_{ji}$ *and* f_{ij} *is an arbitrary constant tensor.*

Proof. According to Noether's theorem for a tensorial field under an r-parameter family of transformations, the variational conservation laws can be expressed in the general form,

$$\frac{\mathrm{d}C_{k\alpha}}{\mathrm{d}x_k} = 0, \quad \alpha = 1,2,\ldots,r, \tag{31}$$

where the conserved quantity is

$$C_{k\alpha} = \left(W^{(2)}\delta_{k\ell} - \beta^{\mathrm{e}}_{ij,\ell}\frac{\partial W^{(2)}}{\partial\beta^{\mathrm{e}}_{ij,k}}\right)\varphi_{\ell\alpha} + \frac{\partial W^{(2)}}{\partial\beta^{\mathrm{e}}_{ij,k}}\xi_{ij\alpha}, \quad k = 1,2,3. \tag{32}$$

We outline the details of the proof as follows:

CL1. *Coordinate translation*: Let $\bar{x}_i = x_i + s_i$ and $\bar{\beta}^{\mathrm{e}}_{ij} = \beta^{\mathrm{e}}_{ij}$ for a vector s_i, as in Li et al. (2006). The corresponding infinitesimal generators for $\alpha = 1,2,3$ are

$$\varphi_{i\alpha} = \left.\frac{\partial\bar{x}_i}{\partial s_\alpha}\right|_{\mathbf{s}=0} = \delta_{i\alpha} \quad \text{and} \quad \xi_{ij\alpha} = \left.\frac{\partial\bar{\beta}^{\mathrm{e}}_{ij}}{\partial s_\alpha}\right|_{\mathbf{s}=0} = 0. \tag{33}$$

One may verify that the r-invariant conditions (Li et al., 2006)

$$\left\{\frac{\partial W^{(2)}}{\partial x_i}\varphi_{i\alpha}+\frac{\partial W^{(2)}}{\partial\beta^{\mathrm{e}}_{ij}}\xi_{ij\alpha}+\frac{\partial W^{(2)}}{\partial\beta^{\mathrm{e}}_{ij,k}}\left(\frac{\mathrm{d}\xi_{ij\alpha}}{\mathrm{d}x_k}-\beta^{\mathrm{e}}_{ij,\ell}\frac{\mathrm{d}\varphi_{\ell\alpha}}{\mathrm{d}x_k}\right)\right\}+W^{(2)}\frac{\mathrm{d}\varphi_{i\alpha}}{\mathrm{d}x_i}=0,$$
$$\forall\mathbf{x}\in\Omega\quad\text{and}\quad\alpha=1,2,\ldots,r \tag{34}$$

are satisfied under coordinate translation. The conserved quantity $S_{k\alpha}$ and the corresponding path-independent integral L_α due to coordinate translation are then given as

$$S_{k\alpha}=W^{(2)}\delta_{k\alpha}-e_{kmi}K_{jm}\beta^{\mathrm{e}}_{ij,\alpha}\rightarrow L_\alpha=\oint_S S_{k\alpha}n_k\,\mathrm{d}S. \tag{35}$$

Remark 4. Since the energy momentum tensor (22) can be derived by a coordinate translation starting from the strain energy density we denote the new conserved quantity $S_{k\alpha}$, which is also obtained due to a coordinate translation, but now starting from compatibility, as the *compatibility momentum tensor*.

CL2. *Coordinate rotation*: Let $\bar{x}_i=Q_{ji}(\mathbf{s})x_j$ and $\bar{\beta}^{\mathrm{e}}_{ij}=Q_{ki}(\mathbf{s})\beta^{\mathrm{e}}_{k\ell}Q_{\ell j}(\mathbf{s})$, for the rotation matrix $\{Q_{ij}(\mathbf{s})\}\in SO(3)$ with $\{Q_{ij}(0)\}=\{\delta_{ij}\}$. For an infinitesimal rotation Q_{ij} is given as

$$Q_{ij}(\mathbf{s})=\delta_{ij}+e_{ijk}s_k+o(\mathbf{s}),\quad k=1,2,3. \tag{36}$$

The corresponding infinitesimal generators for $\alpha=1,2,3$ are

$$\varphi_{i\alpha}=\left.\frac{\partial\bar{x}_i}{\partial s_\alpha}\right|_{\mathbf{s}=0}=\left.\frac{\partial Q_{ji}}{\partial s_\alpha}\right|_{\mathbf{s}=0}x_j=e_{ji\alpha}x_j, \tag{37}$$

$$\xi_{ij\alpha}=\left.\frac{\partial\bar{\beta}^{\mathrm{e}}_{ij}}{\partial s_\alpha}\right|_{\mathbf{s}=0}=\left.\frac{\partial Q_{ki}}{\partial s_\alpha}\right|_{\mathbf{s}=0}\beta^{\mathrm{e}}_{k\ell}Q_{\ell j}|_{\mathbf{s}=0}+Q_{ki}|_{\mathbf{s}=0}\beta^{\mathrm{e}}_{k\ell}\left.\frac{\partial Q_{\ell j}}{\partial s_\alpha}\right|_{\mathbf{s}=0}=e_{ki\alpha}\beta^{\mathrm{e}}_{kj}+e_{\ell j\alpha}\beta^{\mathrm{e}}_{i\ell}. \tag{38}$$

One may verify that the r-invariant conditions (34) are satisfied under coordinate rotation. The conserved quantity $T_{k\alpha}$ and the corresponding path-independent integral F_α due to coordinate rotation are then given as

$$T_{k\alpha}=W^{(2)}e_{jk\alpha}x_j+e_{pki}K_{jp}(e_{m\ell\alpha}x_m\beta^{\mathrm{e}}_{ij,\ell}-e_{mj\alpha}\beta^{\mathrm{e}}_{im})+\delta_{k\alpha}K_{jm}\beta^{\mathrm{e}}_{mj}-K_{j\alpha}\beta^{\mathrm{e}}_{kj}$$
$$\rightarrow F_\alpha=\oint_S T_{k\alpha}n_k\,\mathrm{d}S. \tag{39}$$

CL3. *Scaling*: Let $\bar{x}_i=(1+c_1s)x_i$ and $\bar{\beta}^{\mathrm{e}}_{ij}=(1+c_2s)\beta^{\mathrm{e}}_{ij}$, for constants c_1 and c_2. The corresponding infinitesimal generators for $\alpha=1$ are

$$\varphi_{i\alpha}=\left.\frac{\partial\bar{x}_i}{\partial s_\alpha}\right|_{\mathbf{s}=0}=c_1x_i\quad\text{and}\quad\xi_{ij\alpha}=\left.\frac{\partial\bar{\beta}^{\mathrm{e}}_{ij}}{\partial s_\alpha}\right|_{\mathbf{s}=0}=c_2\beta^{\mathrm{e}}_{ij}. \tag{40}$$

By choosing the constant $c_1=1$ and $c_2=-\frac{1}{2}$, one may verify that the r-invariant conditions (34) are satisfied under scaling. The conserved quantity U_k and the corresponding path-independent integral G due to scaling are then given as

$$U_k=W^{(2)}x_k+\tfrac{1}{2}e_{mki}K_{jm}(\beta^{\mathrm{e}}_{ij}+2\beta^{\mathrm{e}}_{ij,\ell}x_\ell)\rightarrow G=\oint_S U_kn_k\,\mathrm{d}S. \tag{41}$$

CL4. *Constant pre-distortion*: Let $\bar{x}_i = x_i$ and $\bar{\beta}^{\mathrm{e}}_{ij} = \beta^{\mathrm{e}}_{ij} + sf_{ij}$, where f_{ij} is an arbitrary constant tensor. The corresponding infinitesimal generators for $\alpha = 1$ are

$$\varphi_{i\alpha} = \left.\frac{\partial \bar{x}_i}{\partial s_\alpha}\right|_{\mathbf{s}=0} = 0 \quad \text{and} \quad \xi_{ij\alpha} = \left.\frac{\partial \bar{\beta}^{\mathrm{e}}_{ij}}{\partial s_\alpha}\right|_{\mathbf{s}=0} = f_{ij}. \tag{42}$$

One may verify that the r-invariant conditions (34) are satisfied under constant pre-distortion. The conserved quantity P_k and the corresponding path-independent integral H_α due to constant pre-distortion are then given as

$$P_k = -e_{mki}K_{jm}f_{ij} = \left(\frac{1}{2}e_{jki}\alpha_{mm} - e_{mki}\alpha_{mj}\right)f_{ij} \rightarrow H = \oint_S P_k n_k \,\mathrm{d}S. \quad \square \tag{43}$$

Remark 5. As it will be outlined in detail in Section 4, one possible application of the developed compatibility conservation laws in this section can be obtained by combining them with results obtained from conservation laws (22) stemming from equilibrium. As a first immediate consequence of this merging we will point out a possible application of conservation law **CL4** in this remark:

(a) We can choose the arbitrary constant tensor f_{ij} to be $f_{ij} = \sigma_{ij}$ in (43) and note that the dislocation density α_{mj} is given as $\alpha_{mj} = \langle t_m \rangle b_j$ (El-Azab, 2000; Kröner, 2001; Hartley, 2003), where $\langle t_m \rangle$ is the ensemble average of the unit vectors of many distributed dislocation lines, and b_j is the Burgers' vector. Now suppose the stress is symmetric. We then have $\sigma_{ij}e_{jki}\alpha_{mm} = 0$ and (43) reduces to

$$P_k = e_{kmi}\langle t_m \rangle \sigma_{ij} b_j. \tag{44}$$

If we denote $g_i := \sigma_{ij} b_j$, (44) can be written as

$$\mathbf{P} = \langle \mathbf{t} \rangle \times \mathbf{g}, \tag{45}$$

which can be recognized as the Peach–Koehler force written in terms of the ensemble average of the unit vectors of the distributed dislocation lines. Therefore, the physical meaning of conservation law **CL4** for this special case is a well-known result. If the external stress field is constant, any contour integral of the Peach–Koehler force will be zero,

$$H = \oint_S \mathbf{P} \cdot \mathbf{n} \,\mathrm{d}S = 0. \tag{46}$$

This result indicates that the Peach–Koehler force can be derived based on the concept of configurational compatibility. A different recent derivation of the Peach–Koehler force can be found in Lazar and Kirchner (2006).

(b) If the Cauchy stress σ_{ij} is not symmetric as in Toupin (1962), we obtain a generalized version of the Peach–Koehler force as

$$P_k = \tfrac{1}{2} e_{jki}\sigma_{ij} \langle t_m \rangle \, b_m + e_{kmi} \langle t_m \rangle \, \sigma_{ij} b_j. \tag{47}$$

(c) For the case of a single dislocation line, the dislocation density takes the form (Kröner, 2001)

$$\alpha_{mj} = t_m b_j \delta(\rho), \tag{48}$$

where $\delta(\rho)$ is the one-dimensional Dirac's delta function and ρ is the shortest distance from a point to the dislocation line. Therefore, the analogous expression to (45), now in terms of the delta function, is given as

$$\mathbf{P} = \mathbf{t} \times \mathbf{g}\delta(\rho). \tag{49}$$

Under the constant external stress field the analogous expression to (46) is now given as

$$H = \sum_{D} \mathbf{t} \times \mathbf{g} \cdot \mathbf{n} = 0, \tag{50}$$

where D is a set of points at which the dislocation line intercepts the surface S. This is a more familiar form of the Peach–Koehler identity.

To this end, we have constructed the corresponding class of conservation laws based on the defect potential in terms of the dislocation density α_{ij} and the contortion K_{ij}. This was achieved by application of Noether's theorem to the corresponding Lagrangian based on chosen symmetry groups of the system. These conservation laws are derived solely based on kinematic arguments and belong to the introduced concept of configurational compatibility, the dual to the concept of configurational force. In the next section, we employ the developed defect potential and the results of configurational compatibility to derive a multiscale energy momentum tensor.

4. Multiscale energy momentum tensors

The proposed defect potential (24) provides the basis for the construction of the multiscale energy momentum tensor. Although the defect potentials proposed in Remark 1 are kinematic, their corresponding defect energy densities are frequently used in the study of elastoplasticity, including strain gradient plasticity. Steinmann (1996), Kröner (2001), Regueiro et al. (2002), Gurtin (2002), and Clayton et al. (2004) advocate a quadratic form of the defect energy density $\frac{1}{2}A(\ell)\alpha_{ij}\alpha_{ij}$ where α_{ij} is the geometrically necessary dislocation density and $A(\ell)$ is an ad hoc material constant containing a characteristic length scale ℓ. The defect energy represents the stored elastic energy from geometrically necessary dislocations. Because the Euler–Lagrange equations of the defect potential $\frac{1}{2}\alpha_{ij}K_{ji}$, used in the development of the concept of configurational compatibility in Section 3, contain the quadratic form as a special case, we propose using the defect energy density $\frac{1}{2}A(\ell)\alpha_{ij}K_{ji}$ to characterize the fine scale stored elastic energy. Given a variationally consistent defect energy density, we can employ a multiscale variational principle to construct a fine scale contribution to the energy momentum tensor.

4.1. The multiscale variational principle and corresponding Euler–Lagrange equations

We first construct a multiscale energy density following a proposal suggested by Kröner (2001) as

$$W^{(m)} := W^{(1)} + \tilde{W}^{(2)}, \tag{51}$$

where the strain energy density $W^{(1)}$ is denoted as the coarse scale energy density and $\tilde{W}^{(2)} := A(\ell)W^{(2)}$, with the defect potential $W^{(2)}$ given in (24), is called the fine scale energy density. Steinmann (1996) suggested the following form of $A(\ell)$, namely $A(\ell) = \mu\ell^2$, where μ is the shear modulus, so that $\tilde{W}^{(2)}$ has units of energy density. Again, we note that the proposed theory is restricted to infinitesimal deformations. The fine scale energy density defines a "*moment stress*" (Kröner, 2001)

$$\tau_{ij} = A(\ell)K_{ij}. \tag{52}$$

Then the stationary conditions $\delta_u \Pi^{(m)} = 0$ and $\delta_{\beta^e}\Pi^{(m)} = 0$ of the following two-field multiscale mixed variational principle,

$$\Pi^{(m)}(\mathbf{u}, \boldsymbol{\beta}^e) := \int_\Omega W^{(m)}(\nabla\mathbf{u}, \boldsymbol{\beta}^e_{,i})\,\mathrm{d}\Omega, \tag{53}$$

provided that u_i and β^e_{ij} are prescribed on the boundary $\partial\Omega$, results in the Euler–Lagrange equations

$$\delta_u \Pi^{(m)} = 0 \to C_{ijk\ell}u_{\ell,ki} = 0 \quad \forall \mathbf{x} \in \Omega \text{ and } u_i = \bar{u}_i \;\; \forall \mathbf{x} \in \partial\Omega, \tag{54}$$

$$\delta_{\beta^e}\Pi^{(m)} = 0 \to -e_{ik\ell}K_{j\ell,k} = 0 \quad \forall \mathbf{x} \in \Omega \text{ and } \beta^e_{ij} = \bar{\beta}^e_{ij} \;\; \forall \mathbf{x} \in \partial\Omega. \tag{55}$$

Both, the coarse scale (equilibrium) and the fine scale (compatibility) contribute to the multiscale variational principle.

4.2. Derivation of the multiscale energy momentum tensor

Based on the Lagrangian (54)–(55) we will derive now the corresponding multiscale energy momentum tensor by applying Noether's theorem for the case of a coordinate translation.

Theorem 6. *Consider a simply connected continuum under infinitesimal deformation. Let* $\Omega \in \mathbb{R}^3$ *with Lipschitz continuous boundary* $\partial\Omega$. *Assume that the displacement* $u_i(\mathbf{x})$ *satisfies the vectorial differential equation* (54) *and assume that the elastic distortion* $\beta^e_{ij}(\mathbf{x})$ *satisfies the tensorial differential equations given in* (55). *Then, based on the result of Noether's theorem for a vectorial and tensorial field* (Li et al., 2006), *the following conservation law holds together with its path-independent integral*:

$$\mathscr{S}^{(m)}_{k\alpha} = (W^{(1)}\delta_{k\alpha} - u_{\ell,\alpha}\sigma_{k\ell}) + (\tilde{W}^{(2)}\delta_{k\alpha} - e_{kmi}\beta^e_{ij,\alpha}\tau_{jm}) =: E_{k\alpha} + \tilde{S}_{k\alpha}, \tag{56}$$

$$\mathscr{L}^{(m)}_\alpha = \oint_S \mathscr{S}^{(m)}_{k\alpha} n_k\,\mathrm{d}S =: J_\alpha + \tilde{L}_\alpha, \tag{57}$$

where $W^{(1)} = \frac{1}{2}\sigma_{ij}\varepsilon_{ij}$ *and* $\tilde{W}^{(2)} = \frac{1}{2}\alpha_{ij}\tau_{ji}$.

Proof. According to Noether's theorem, the variational conservation laws can be expressed in the general form,

$$\frac{\mathrm{d}C^{(m)}_{k\alpha}}{\mathrm{d}x_k} = 0, \quad \alpha = 1, 2, \ldots, r, \tag{58}$$

where the conserved quantity is

$$C^{(m)}_{k\alpha} = \left(W^{(1)}\delta_{k\ell} - u_{i,\ell}\frac{\partial W^{(1)}}{\partial u_{i,k}}\right)\varphi_{\ell\alpha} + \frac{\partial W^{(1)}}{\partial u_{i,k}}\xi_{i\alpha} + \left(\tilde{W}^{(2)}\delta_{k\ell} - \beta^e_{ij,\ell}\frac{\partial \tilde{W}^{(2)}}{\partial \beta^e_{ij,k}}\right)\varphi_{\ell\alpha} + \frac{\partial \tilde{W}^{(2)}}{\partial \beta^e_{ij,k}}\xi_{ij\alpha}, \quad k = 1, 2, 3. \tag{59}$$

Under coordinate translation we let $\bar{x}_i = x_i + s_i$, $\bar{u}_i = u_i$, and $\bar{\beta}^{\mathrm{e}}_{ij} = \beta^{\mathrm{e}}_{ij}$. Then the corresponding infinitesimal generators for $\alpha = 1, 2, 3$ are

$$\varphi_{i\alpha} = \left.\frac{\partial \bar{x}_i}{\partial s_\alpha}\right|_{\mathbf{s}=0} = \delta_{i\alpha}, \quad \xi_{i\alpha} = \left.\frac{\partial \bar{u}_i}{\partial s_\alpha}\right|_{\mathbf{s}=0} = 0 \quad \text{and} \quad \xi_{ij\alpha} = \left.\frac{\partial \bar{\beta}^{\mathrm{e}}_{ij}}{\partial s_\alpha}\right|_{\mathbf{s}=0} = 0. \tag{60}$$

One may verify that the r-invariant conditions (34) are satisfied under coordinate translation. We then obtain the multiscale energy momentum tensor $\mathscr{S}^{(m)}_{k\alpha}$ and the corresponding path-independent integral $\mathscr{L}^{(m)}_{\alpha}$ given in (56) and (57), respectively. □

In (56) we interpret Eshelby's energy momentum tensor $E_{k\alpha}$ as the coarse scale contribution and the scaled compatibility momentum tensor $\tilde{S}_{k\alpha} := A(\ell)S_{k\alpha}$ as the fine scale contribution. The coarse scale and fine scale counterparts in (57) are denoted as J_α and $\tilde{L}_\alpha := A(\ell)L_\alpha$, respectively. Similar to the coarse scale driving force J_α, we interpret $\tilde{L}_\alpha$ as a fine scale driving force acting on the defect. The fine scale driving force derived here is a configurational force acting on a collective defect, a collection of geometrically necessary dislocations. $\mathscr{S}^{(m)}_{k\alpha}$ is divergence-free and $\mathscr{L}^{(m)}_{\alpha}$ is path-independent if the solid is defect-free.

We would like to stress the fact that the multiscale energy density does not coincide with the total potential energy density of a solid with a particular constitutive relation. The fine scale energy density was not derived from a fine scale constitutive theory. Instead, it is a defect energy density expressed in terms of a defect potential that reflects the density of geometrically necessary dislocations. In fact, a defect energy, such as lattice misfit energy density, has already been used to derive lattice resistance stresses or forces, such as the Peierls potential or the Peierls energy (Peierls, 1940; Nabarro, 1952). The defect energy density constructed here is not for a single dislocation but for a geometrically necessary dislocation distribution based on the continuum dislocation theory. We furthermore stipulate that the moment stresses generated by our formulation do not enter the coarse scale balance laws and that the derivation of the defect potential does not rely on balance laws at the fine scale. The fine scale energy density stems from configurational compatibility.

5. Application to an example of a mode III elasto-plastic crack problem

In this section, the concepts of configurational compatibility and multiscale energy momentum tensors are applied to an example of a mode III elasto-plastic crack problem.

The Hult–McClintock solution (Hult and McClintock, 1957; Rice, 1967) for the mode III crack in an elastic perfectly-plastic medium, illustrated in Fig. 1, is considered in the analysis. In the case of small-scale yielding, the plastic zone Ω_{p} is assumed much smaller than the crack length a. The shape of the plastic zone Ω_{p}, illustrated in Fig. 1, is a circular region ahead of the crack tip. The applied stress intensity is $K_{\mathrm{III}} = \sqrt{a\pi}\tau_\infty$ where τ_∞ is the applied, far-field stress. One may employ a matching condition to determine the size of the plastic zone,

$$r_0 = \frac{K_{\mathrm{III}}^2}{2\pi\tau_0^2} = \frac{a}{2}\left(\frac{\tau_\infty}{\tau_0}\right)^2, \tag{61}$$

where τ_0 is the shear yield stress. The small-scale yielding assumption $r_0/a \ll 1$ is valid when $\tau_\infty/\tau_0 \ll 1$. The center of the plastic zone is at a distance r_0 ahead of the crack tip. All the

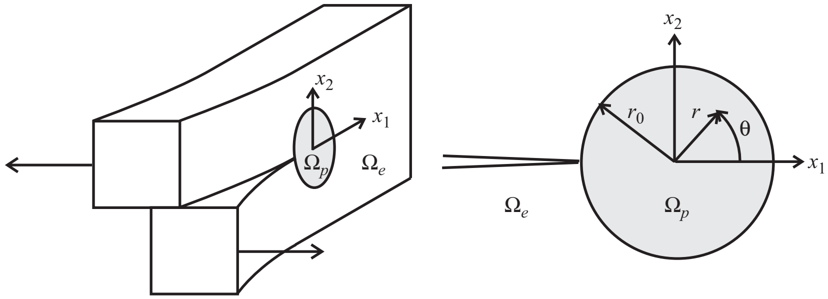

Fig. 1. Illustration of a mode III crack in an elastic perfectly-plastic medium. The circular plastic zone Ω_p is located ahead of the crack tip with radius r_0.

Table 1
Field quantities in the elastic region Ω_e and the plastic region Ω_p

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

needed field quantities for both the linear elastic region Ω_e and the perfectly plastic region Ω_p are given in Table 1. Note that because only $u_3 \neq 0$, we can easily calculate the elastic distortion tensor $\boldsymbol{\beta}^\mathrm{e}$ through the elastic strain tensor $\boldsymbol{\varepsilon}^\mathrm{e}$ taken from the stress tensor $\boldsymbol{\sigma}$.

5.1. *Application of configurational compatibility*

The importance of the J-integral in linear elastic fracture mechanics motivates the application of the new path-independent integrals derived from the defect potential (24). The compatibility momentum tensor and corresponding path-independent integral **CL1**, given in (27), are calculated for the mode III elasto-plastic crack to improve our understanding of the derived quantities.

Equipped with the needed kinematics given in Table 1, we can calculate the individual components of the compatibility momentum tensor and its path-independent integral. The dislocation density $\boldsymbol{\alpha}$ as well as the contortion $\mathbf{K}$ are zero in the elastic region Ω_e and the only non-zero component of $\boldsymbol{\alpha}$ in the plastic region Ω_p is

$$\alpha_{33} = -\frac{\tau_0}{2r\mu}\cos\frac{\theta}{2} \quad \forall \mathbf{x} \in \Omega_p, \tag{62}$$

from which also the contortion $\mathbf{K}$ in the plastic region Ω_p can be easily computed. Further calculations yield to the configurational compatibility tensor $\mathbf{S}$ and the corresponding contour integral $\mathbf{L}$ as

$$\mathbf{S} = \frac{\tau_0^2}{32r^2\mu^2}\begin{bmatrix} -2\cos^2\frac{\theta}{2}(1-2\cos\theta) & \sin 2\theta & 0 \\ 4\cos^2\frac{\theta}{2}\sin\theta & 2\cos^2\frac{\theta}{2}(1-2\cos\theta) & 0 \\ 0 & 0 & 2\cos^2\frac{\theta}{2} \end{bmatrix} \quad \forall \mathbf{x} \in \Omega_p \tag{63}$$

and

$$\mathbf{L} = \frac{3\pi\tau_0^2}{32r_0\mu^2}\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \quad \forall \mathbf{x} \in \Omega_p. \tag{64}$$

The integral is evaluated at the boundary of the plastic zone r_0, which is in contrast to the earlier studies of dislocation emission at the crack tip. Rather than focus on a single dislocation positioned at a particular orientation, the $\mathbf{L}$-integral provides an integrated measure of configurational incompatibility. Note that we did not express either $\mathbf{S}$ or $\mathbf{L}$ in the compatible, elastic field because all contour integrals will yield a null measure. Therefore, any contour integrals outside the plastic zone will be path-independent

$$\mathbf{L} = \oint_S \mathbf{n}\cdot\mathbf{S}\,\mathrm{d}S = \mathbf{0}, \tag{65}$$

whereas inside the plastic zone, the configurational integral is not invariant. The elastic strain field inside the plastic zone is not compatible and results in a non-zero geometrically necessary dislocation density $\boldsymbol{\alpha}$ of screw type ($\alpha_{33} \neq 0$). The non-zero $\mathbf{L}$-integral encircling the incompatible, plastic region provides a measure of incompatibility.

5.2. Application of multiscale energy momentum tensors

Calculation of the multiscale energy momentum tensor $\mathscr{S}^{(m)}_{k\alpha}$ and corresponding configurational force $\mathscr{L}^{(m)}_\alpha$ is straightforward. Given in (57), $\mathscr{L}^{(m)}_\alpha$ is composed of a coarse scale component $\mathbf{J}$ and a fine scale component $\tilde{\mathbf{L}}:=A(\ell)\mathbf{L}$ with $\mathbf{L}$ given in (64) for the example of a mode III elasto-plastic crack. $\mathscr{L}^m$ can then be written as

$$\mathscr{L}^m = \begin{bmatrix} \frac{K_{\mathrm{III}}^2}{2\mu} \\ 0 \\ 0 \end{bmatrix} + A(\ell)\begin{bmatrix} \frac{3\pi\tau_0^2}{32r_0\mu^2} \\ 0 \\ 0 \end{bmatrix}. \tag{66}$$

The first term is the familiar J-integral for mode III propagation. The second term is the configurational force stemming from incompatibility. We assume the form of $A(\ell)$ to be $\mu\ell^2$ where μ is the shear modulus and ℓ is the length scale governing incompatibility. Taking the first component of $\mathscr{L}^m$, denoting it as L^m and making use of (61), we express the multiscale driving force as a function of the applied loading τ_∞ and the crack geometry a as

$$L^m = \left(\frac{\pi\tau_\infty^2}{2\mu}\right)a + \left(\frac{3\ell^2\pi\tau_0^4}{16\mu\tau_\infty^2}\right)\frac{1}{a} =: J + \tilde{L}, \tag{67}$$

where we introduced $\tilde{L} := A(\ell)L = \mu\ell^2 L$ where L is the first component of $\mathbf{L}$. Let us normalize the multiscale driving force L^m by J to obtain

$$\frac{L^m}{J} = 1 + \frac{1}{(a/a_{\min})^2} \quad \text{with } a_{\min} := \sqrt{\frac{3}{8}}\left(\frac{\tau_0}{\tau_\infty}\right)^2 \ell. \tag{68}$$

In Fig. 2, the normalized multiscale driving force L^m/J is plotted against the normalized crack length $a/a_{\min}$. One can observe that as $a \gg a_{\min}$, $L^m \to J$, which implies that for macroscopic crack lengths, the driving force for brittle fracture is controlled by J. In contrast, for $a \sim a_{\min}$, the fine scale driving force will dominate and result in a multiscale driving force that is larger than the coarse scale driving force J. We also note that the fine scale contributions to (51) and (67) scale with ℓ. As $\ell \to 0$, the multiscale driving force L^m collapses onto the classical coarse scale driving force J.

In order to discuss the physical meaning of the introduced quantity $a_{\min}$, we perform a stability analysis of the multiscale driving force L^m. For brittle fracture, we may assume a constant fracture resistance $2\gamma_t$, so $\partial(2\gamma_t)/\partial a = 0$. Thus $\partial L^m/\partial a < 0$ implies stable crack

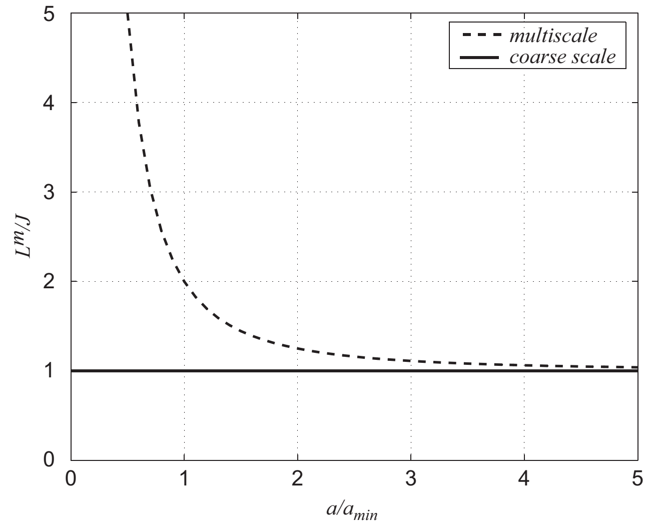

Fig. 2. The normalized multiscale driving force L^m/J versus the normalized crack length $a/a_{\min}$. As $a \gg a_{\min}$ the multiscale driving force L^m approaches the coarse scale driving force J.

growth. The minimum may be found via the stationary condition

$$\left.\frac{\partial L^m}{\partial a}\right|_{\tau\infty} = \left(\frac{\pi\tau_\infty^2}{2\mu}\right) - \left(\frac{3\ell^2\pi\tau_0^4}{16\mu\tau_\infty^2}\right)\frac{1}{a^2} = 0. \tag{69}$$

Therefore, the minimum driving force to advance a crack and the stability point are given as

$$L_{\min}^m = \sqrt{\frac{3}{2}}\frac{\pi\ell\tau_0^2}{2\mu} = \frac{\pi\tau_\infty^2}{\mu}a_{\min} \quad \text{at } a = a_{\min}. \tag{70}$$

The introduced quantity $a_{\min}$, used to express the normalized multiscale driving force in (68), represents the crack length at instability. These findings indicate that an incompatible field will yield a minimum driving force. In addition, incompatibility enables stable crack growth under load control for $a < a_{\min}$.

In order to obtain an illustration of the stability analysis, we normalize the multiscale driving force L^m by its minimum value $L_{\min}^m$ and obtain

$$\frac{L^m}{L_{\min}^m} = \frac{a}{2a_{\min}} + \frac{1}{2a/a_{\min}}. \tag{71}$$

In Fig. 3, we plot this normalization of the multiscale driving force against the normalized crack length $a/a_{\min}$. It can be seen from Fig. 3 that there is a well-located minimum at $a = a_{\min}$. This suggests that the driving force for crack growth cannot be zero, even if the crack length a approaches zero. The reason for this is due to the fact that the total energy release rate has two sources, namely (1) the coarse scale energy release rate derived from the strain energy $W^{(1)}$ and (2) the fine scale energy release rate derived from the defect energy $\tilde{W}^{(2)}$. In this work, the fine scale defect energy represents the stored energy from a collection of geometrically necessary dislocations.

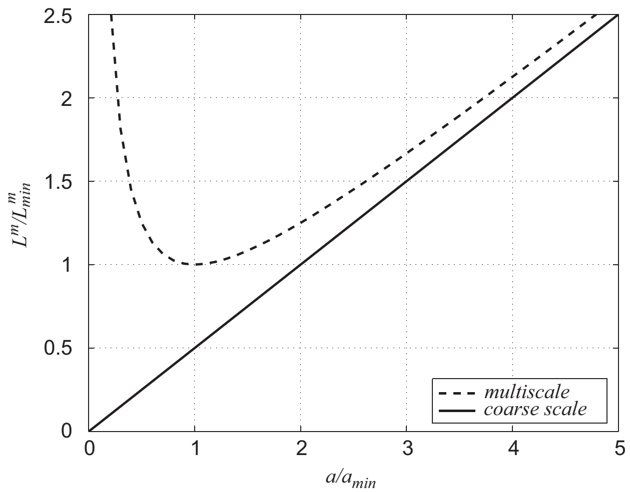

Fig. 3. The normalized crack driving force $L^m/L_{\min}^m$ versus the normalized crack length $a/a_{\min}$. Contrary to the coarse scale driving force J, the multiscale driving force L^m reaches a non-zero minimum at $a = a_{\min}$.

6. Closure

In this paper the multiscale phenomena of brittle fracture have been discussed. This was achieved through the introduction of a concept termed *configurational compatibility* dual to the concept of configurational force. The framework of configurational compatibility was built upon the construction of a valid defect potential in terms of the dislocation density and the contortion. Application of Noether's theorem yielded a new class of compatibility conservation laws. It was shown that the Peach–Koehler force can be viewed as a special case of one of the derived compatibility conservation laws. We argued that the conservation laws stemming from configurational compatibility will be valid for any continuum independent of constitution. In contrast to classical continuum conservation laws based on equilibrium conditions, kinematic conservation laws are valid at a smaller length scale. Based on the proposed defect potential and its corresponding defect energy, a two-field multiscale mixed variational principle was employed to construct a *multiscale energy momentum tensor*. We showed that the multiscale energy momentum tensor is composed of a coarse scale component, Eshelby's energy momentum tensor, and a fine scale component, a scaled compatibility momentum tensor. We then applied the new framework to the example of a mode III elasto-plastic crack and illustrated that incompatibility yielded a minimum driving force.

Not all the possible defect potentials and compatibility conservation laws have been exhausted in this work. There may exist other forms of defect potentials and corresponding conservation laws which will be explored in a subsequent work. The discovery and interpretation of the kinematic conservation laws might enable new physical concepts and improvements in material science. The understanding of the physical meaning of the derived conservation laws needs to be improved and the multiscale energy momentum tensors should be applied to additional realistic examples.

Acknowledgments

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