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Dislocation equilibrium conditions revisited

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Abstract

If there is an equilibrium arrangement of a given collection of dislocations, each having a fixed size and shape, in an externally loaded or unloaded elastic body, the corresponding potential energy will be stationary with respect to infinitesimal perturbations of the dislocation positions. This leads to the dislocation equilibrium conditions: the Peach–Koehler forces along the dislocation line of each dislocation due to externally applied stress and the interaction of the dislocation with other dislocations and its own image field is a set of self-equilibrated forces. The earlier proof of this result presented in the literature was based on an incomplete expression for the elastic strain energy. This is modified here by using the elastic strain energy expression that accounts for all dislocation core energy.

Keywords: Core energy; Dislocation equilibrium; Dislocation interactions; Peach–Koehler force; Potential energy; Strain energy; Variational principle

1. Introduction

A significant progress has been made during the past fifteen years in the development of a dislocation-based plasticity theory and the analysis of its relationship to various phenomenological continuum plasticity theories (Gulluoglu et al., 1989; Amodeo and Ghoniem, 1990a,b; Kubin et al., 1992; Van der Giessen and Needleman, 1995; Cleveringa et al., 1999; Zbib et al., 1998, 2002; Needleman and Van der Giessen, 2001; Deshpande et al., 2003; Ghoniem et al., 2003; Acharya, 2004). In a dislocation-based analysis plastic deformation is viewed to be a consequence of the collective motion of large numbers of dislocations described as line defects in an elastic body. Toward this analysis, Lubarda et al. (1993) studied the equilibrium arrangements of dislocations in an externally unloaded elastic body by finding the configurations that

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minimize the elastic strain energy with respect to infinitesimal variations of the dislocation positions. The corresponding dislocation equilibrium conditions were that the Peach–Koehler forces along each dislocation line, due to its interaction with other dislocations and its own image field, represent a set of the self-equilibrated forces. This result was derived in their paper by using an expression for the elastic strain energy which only partly accounted for the elastic core energies. The derivation is modified here by using a complete expression for the elastic strain energy that, in principle, accounts for all dislocation core energy. The potential energy expression for the dislocations in an externally loaded or constrained body, with the corresponding conditions for the equilibrium dislocation configurations, are also derived. In addition to dislocations with a fixed size and shape, the presented analysis may also be of interest to study the equilibrium or moving configurations of dislocations that can change their size and shape, for which the self-energies of individual dislocation loops and the interaction of dislocation segments among themselves play an important role.

2. Elastic strain energy of a dislocated body

Consider an externally unloaded body of volume V bounded by the surface S. The body is in the state of a self-equilibrated stress $\boldsymbol{\sigma}$ and the corresponding strain $\boldsymbol{\epsilon}$, which are produced by a given distribution of n planar dislocation loops, as sketched in Fig. 1a. Each dislocation is created by making a planar cut within the loop L^i and displacing the lower face of the cut relative to the upper face by the constant Burgers vector $\mathbf{b}^i$, i.e.,

$$\mathbf{u}_{A^i_-} - \mathbf{u}_{A^i_+} = \mathbf{b}^i, \quad i = 1, 2, \ldots, n. \tag{1}$$

The outward unit normal to the lower face of the cut A^i_- is $\mathbf{n}^i$. The elastic stress and strain fields are independent of the choice of an open surface emanating from L^i across which the displacement discontinuity is imposed to create a dislocation, so that the planar cuts are selected for convenience (or to make the contact with the crystalline dislocations for which the slip occurs across the crystallographic planes).[1] Since elastic stress and strain fields become singular at the points of a dislocation loop due to the self-stress of each dislocation (the strength of the singularity being $1/r$, where r is the distance from the loop), the total elastic strain energy will be formally infinitely large. If we imagine, as in Gavazza and Barnett (1976), that a dislocation core—a small toroidal region V^i_{core} around each dislocation loop, is removed from the body, the elastic strain energy in the remaining part of the body (Fig. 1b), having the volume V_0, is

$$U_0 = \frac{1}{2}\int_{V_0} \boldsymbol{\sigma} : \boldsymbol{\epsilon}\,\mathrm{d}V = \frac{1}{2}\sum_{i=1}^{n}\int_{S^i} \mathbf{T}\cdot\mathbf{u}\,\mathrm{d}S + \frac{1}{2}\sum_{i=1}^{n}\int_{A^i_0} \mathbf{n}^i\cdot\boldsymbol{\sigma}\cdot\mathbf{b}^i\,\mathrm{d}A. \tag{2}$$

This directly follows from the Gauss divergence theorem. The traction vector over the inner surface S^i of the tube is $\mathbf{T} = \boldsymbol{\upsilon}^i\cdot\boldsymbol{\sigma}$ and the associated displacement vector is $\mathbf{u}$. The second surface integral in (2) is the work of the traction $\mathbf{n}^i\cdot\boldsymbol{\sigma}$ on the slip discontinuity $\mathbf{b}^i$ across the area $A^i_0 = A^i - A^i_{\text{core}}$ within each loop L^i outside the core region (Fig. 2b). The elastic strain energy in the whole body, including the core regions, is

$$U = U_0 + \sum_{i=1}^{n} U^i_{\text{core}} = \frac{1}{2}\int_{V_0} \boldsymbol{\sigma} : \boldsymbol{\epsilon}\,\mathrm{d}V + \sum_{i=1}^{n} U^i_{\text{core}}. \tag{3}$$

Within the linear elastic theory and the Volterra type dislocations (constant Burgers vector everywhere within the loop), the core energies U^i_{core} are unbounded due to divergent self-stress and strain fields of each dislocation at the points of the loop. However, as will be shown in Section 3, for the fixed size and shape of

[1] For dislocations in multiply connected bodies, see Lubarda (1999) and Lubarda and Markenscoff (2003).

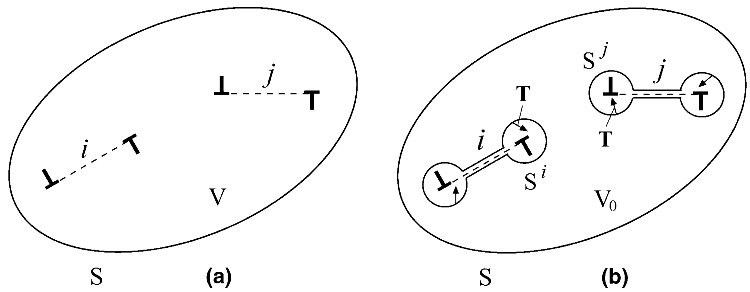

Fig. 1. (a) Dislocation loops within the body of volume V bounded by the surface S. (b) The volume V_0 outside the core regions of the dislocations. The traction vector over the internal core surface S^i is $\mathbf{T}$.

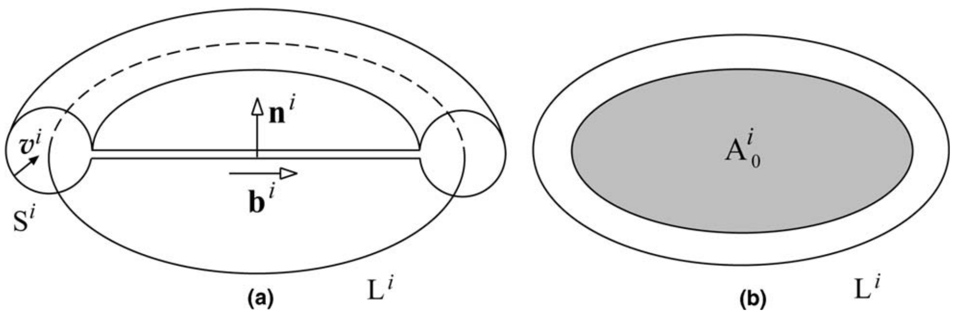

Fig. 2. (a) The toroidal core region around the dislocation line L^i with the Burgers vector $\mathbf{b}^i$. For a glide dislocation $\mathbf{b}^i$ is in the plane of the loop. (b) The slip area A_0^i within the dislocation loop outside the core region.

the loops, the variational procedure based on $\delta U = 0$ outfaces the divergent part of $U_{\rm core}^i$, delivering the dislocation equilibrium conditions independently of the singularity inherent in an idealized Volterra dislocation model.

Lubarda et al. (1993), and Van der Giessen and Needleman (1995), considered the dislocation core energies to be equal to the work done by the tractions $(-\mathbf{T})$, acting over external surfaces of the extracted toroidal cores, on the corresponding displacements $\mathbf{u}$, i.e.,

$$\sum_{i=1}^{n} U_{\rm core}^i = \frac{1}{2}\sum_{i=1}^{n}\int_{S^i}(-\mathbf{T})\cdot\mathbf{u}\,{\rm d}S. \tag{4}$$

This expression does not include a (divergent) work contribution associated with the slip discontinuity $\mathbf{b}^i$ across the area $A_{\rm core}^i = A^i - A_0^i$ within the core region (Fig. 3). The complete expression for the core energy is consequently

$$\sum_{i=1}^{n} U_{\rm core}^i = \frac{1}{2}\sum_{i=1}^{n}\int_{S^i}(-\mathbf{T})\cdot\mathbf{u}\,{\rm d}S + \frac{1}{2}\sum_{i=1}^{n}\int_{A_{\rm core}^i}\mathbf{n}^i\cdot\boldsymbol{\sigma}\cdot\mathbf{b}^i\,{\rm d}A, \tag{5}$$

where the second term on the right-hand side is formally infinite for an idealized Volterra dislocation. As discussed in Section 4, if the divergence of the stress and strain fields within the dislocation core is eliminated by using more involved continuum or atomistic models (which take into account the crystallographic structure near the dislocation line), it is found that the calculated core energy is very different from the traction work over the core surface alone (the performed calculations indicate that for glide dislocations the core energy can be five or more times greater than the traction work alone).

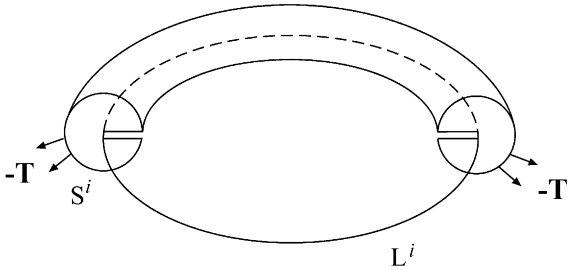

Fig. 3. The extracted core of the dislocation (one half of the core is shown), with the surface traction ($-\mathbf{T}$) acting over its external surface S^i. Also indicated is the cut surface within the core across which the displacement discontinuity is imposed.

Returning to the total elastic strain energy, the expression used by Lubarda et al. (1993) is

$$\overline{U} = \frac{1}{2}\int_{V_0} \boldsymbol{\sigma} : \boldsymbol{\epsilon}\,\mathrm{d}V + \frac{1}{2}\sum_{i=1}^{n}\int_{S^i}(-\mathbf{T})\cdot\mathbf{u}\,\mathrm{d}S = \frac{1}{2}\sum_{i=1}^{n}\int_{A_0^i}\mathbf{n}^i\cdot\boldsymbol{\sigma}\cdot\mathbf{b}^i\,\mathrm{d}A, \tag{6}$$

while the complete expression for the elastic strain energy is

$$U = \frac{1}{2}\sum_{i=1}^{n}\int_{A^i}\mathbf{n}^i\cdot\boldsymbol{\sigma}\cdot\mathbf{b}^i\,\mathrm{d}A = \overline{U} + \frac{1}{2}\sum_{i=1}^{n}\int_{A^i_{\mathrm{core}}}\mathbf{n}^i\cdot\boldsymbol{\sigma}\cdot\mathbf{b}^i\,\mathrm{d}A. \tag{7}$$

The divergent part of the strain energy in the above expression is circumvented by the variational procedure based on $\delta U = 0$, as shown next.

3. Dislocation equilibrium conditions

As in Lubarda et al. (1993) and Lubarda (1993), the stress field in the dislocated body is written as the sum of two fields, $\boldsymbol{\sigma} = \tilde{\boldsymbol{\sigma}} + \hat{\boldsymbol{\sigma}}$. The field $\tilde{\boldsymbol{\sigma}}$ is the infinite medium dislocation field, obtained by the superposition of the stress fields $\tilde{\boldsymbol{\sigma}}^i$ of individual dislocations in an infinite medium, i.e.,

$$\tilde{\boldsymbol{\sigma}} = \sum_{i=1}^{n}\tilde{\boldsymbol{\sigma}}^i. \tag{8}$$

Since $\tilde{\boldsymbol{\sigma}}$ gives rise to surface traction $\widetilde{\mathbf{T}} = \mathbf{n}\cdot\tilde{\boldsymbol{\sigma}}$ over the surface S bounding the volume V within the infinite medium, the other stress field $\hat{\boldsymbol{\sigma}}$ is introduced to cancel this surface traction (image field). Thus,

$$\nabla\cdot\hat{\boldsymbol{\sigma}} = \mathbf{0} \quad \text{in } V, \qquad \mathbf{n}\cdot\hat{\boldsymbol{\sigma}} = -\sum_{i=1}^{n}\widetilde{\mathbf{T}}^i \quad \text{on } S. \tag{9}$$

The sum of the two fields within the volume V defines the stress field of a dislocated body with zero traction over its external surface S. Consequently,

$$\mathbf{n}^i\cdot\boldsymbol{\sigma}\cdot\mathbf{b}^i = \mathbf{n}^i\cdot\hat{\boldsymbol{\sigma}}\cdot\mathbf{b}^i + \sum_{j\neq i}\mathbf{n}^i\cdot\tilde{\boldsymbol{\sigma}}^j\cdot\mathbf{b}^i + \mathbf{n}^i\cdot\tilde{\boldsymbol{\sigma}}^i\cdot\mathbf{b}^i. \tag{10}$$

The substitution of (10) into (6) gives

$$U = \frac{1}{2}\sum_{i=1}^{n}\int_{A^i}\mathbf{n}^i\cdot\left(\hat{\boldsymbol{\sigma}} + \sum_{j\neq i}\tilde{\boldsymbol{\sigma}}^j\right)\cdot\mathbf{b}^i\,\mathrm{d}A + \frac{1}{2}\sum_{i=1}^{n}\int_{A^i}\mathbf{n}^i\cdot\tilde{\boldsymbol{\sigma}}^i\cdot\mathbf{b}^i\,\mathrm{d}A. \tag{11}$$

The integral

$$\widetilde{U}^{i}_{\text{self}} = \frac{1}{2}\int_{A_i} \mathbf{n}^i \cdot \tilde{\boldsymbol{\sigma}}^i \cdot \mathbf{b}^i \, \mathrm{d}A \tag{12}$$

is the self-energy of the ith dislocation in an infinite linearly elastic medium. The far-field displacements and stresses fall off as $1/r^2$ and $1/r^3$, respectively, away from the loop (Hirth and Lothe, 1982), while the dominant stress singularity near the loop is of the order $1/r$. This leads to an unbounded value for $\widetilde{U}^{i}_{\text{self}}$. However, since the self-energy of a dislocation loop in an infinite isotropic medium does not depend on its position or orientation (assuming that the dislocation does not change its size or shape), the variation of $\widetilde{U}^{i}_{\text{self}}$ with respect to the dislocation position is zero,

$$\delta \widetilde{U}^{i}_{\text{self}} = 0. \tag{13}$$

The first term on the right-hand side of (11) is bounded because the stresses within the loop i (including the points of the dislocation line itself) due to the interaction with other loops $j \neq i$ are all finite. Thus, as shown in Appendix A, the variation of the strain energy is

$$\delta U = \sum_{i=1}^{n} \int_{\delta A^i} \mathbf{n}^i \cdot \left(\hat{\boldsymbol{\sigma}} + \sum_{j\neq i} \tilde{\boldsymbol{\sigma}}^j \right) \cdot \mathbf{b}^i \, \mathrm{d}(\delta A). \tag{14}$$

If $\delta \mathbf{x}^i$ is an infinitesimal displacement of the point of the dislocation line associated with the variation of the dislocation position, we have $\mathbf{n}^i \mathrm{d}(\delta A) = \delta \mathbf{x}^i \times \mathrm{d}\mathbf{L}$, where $\mathrm{d}\mathbf{L} = \mathrm{d}L\mathbf{t}$ is an infinitesimal segment of the dislocation line ($\mathbf{t}$ being its unit tangent vector). It readily follows that

$$\delta U = \sum_{i=1}^{n} \int_{L^i} \mathbf{f} \cdot \delta \mathbf{x}^i \, \mathrm{d}L, \tag{15}$$

where

$$\mathbf{f} = \mathbf{t} \times \left(\hat{\boldsymbol{\sigma}} + \sum_{j\neq i} \tilde{\boldsymbol{\sigma}}^j \right) \cdot \mathbf{b}^i \tag{16}$$

is the Peach–Koehler force along the dislocation line L^i due to the interaction of the ith dislocation with all other dislocations and its own image field. Indeed, since $\boldsymbol{\sigma}^i = \hat{\boldsymbol{\sigma}}^i + \tilde{\boldsymbol{\sigma}}^i$, we have

$$\hat{\boldsymbol{\sigma}} + \sum_{j\neq i} \tilde{\boldsymbol{\sigma}}^j = \hat{\boldsymbol{\sigma}}^i + \sum_{j\neq i} \boldsymbol{\sigma}^j = \boldsymbol{\sigma} - \tilde{\boldsymbol{\sigma}}^i. \tag{17}$$

The dislocations within the body V will be in equilibrium if $\delta U = 0$ for any infinitesimal variation of the dislocation positions. Since the variations $\delta \mathbf{x}^i$ are independent, it follows that for each dislocation at equilibrium

$$\int_{L^i} \mathbf{f} \cdot \delta \mathbf{x}^i \, \mathrm{d}L = 0. \tag{18}$$

If the variation of the dislocation position corresponds to a pure translation of the amount δx^i in the unit direction $\mathbf{x}_0$, then $\delta \mathbf{x}^i = \delta x^i \mathbf{x}_0$. Since δx^i and $\mathbf{x}_0$ are arbitrary, Eq. (18) implies that

$$\int_{L^i} \mathbf{f} \, \mathrm{d}L = \mathbf{0}, \tag{19}$$

i.e., the total Peach–Koehler force of each dislocation due to its interaction with other dislocations is equal to zero. If the variation of the dislocation position corresponds to rotation of the amount $\delta\omega^i$ around the unit direction $\mathbf{x}_0$ passing through an arbitrary point P, then $\delta\mathbf{x}^i = \delta\omega^i\mathbf{x}_0 \times (\mathbf{x}^i - \mathbf{x}_P)$. Since $\delta\omega^i$ and $\mathbf{x}_0$ are arbitrary, Eq. (18) implies that

$$\int_{L^i} (\mathbf{x}^i - \mathbf{x}_P) \times \mathbf{f}\,\mathrm{d}L = \mathbf{0}. \tag{20}$$

Thus the resulting moment of the Peach–Koehler forces of each dislocation due to its interaction with other dislocations is equal to zero. Together (19) and (20) imply that the Peach–Koehler forces of each dislocation, due to its interaction with other dislocations and its own image field, represent a set of the self-equilibrated forces.

4. The core energy

The self-energy of an isolated Volterra dislocation loop in an infinite medium is the sum of the strain energy exterior to the toroidal tube surrounding the dislocation line and the (divergent) core energy within the tube,

$$\widetilde{U}^i_{\text{self}} = \frac{1}{2}\int_{S^i} \widetilde{\mathbf{T}}^i \cdot \tilde{\mathbf{u}}^i\,\mathrm{d}S + \frac{1}{2}\int_{A^i_0} \mathbf{n}^i \cdot \tilde{\boldsymbol{\sigma}}^i \cdot \mathbf{b}^i\,\mathrm{d}A + \widetilde{U}^i_{\text{c}}. \tag{21}$$

By comparing (21) with (11), we can formally express the misfit core energy (the energy associated with the slip discontinuity within the core) as

$$\frac{1}{2}\int_{A^i_{\text{core}}} \mathbf{n}^i \cdot \tilde{\boldsymbol{\sigma}}^i \cdot \mathbf{b}^i\,\mathrm{d}A = \frac{1}{2}\int_{S^i} \widetilde{\mathbf{T}}^i \cdot \tilde{\mathbf{u}}^i\,\mathrm{d}S + \widetilde{U}^i_{\text{c}}. \tag{22}$$

For example, for a straight dislocation in an isotropic infinite medium with the Burgers vector $\mathbf{b} = \{b_1, b_2, b_3\}$ (b_3 being its screw component), the work of the tractions over the internal surface of the dislocation core is (for the Volterra dislocation)

$$\frac{1}{2}\int_{S^i} \widetilde{\mathbf{T}}^i \cdot \tilde{\mathbf{u}}^i\,\mathrm{d}S = \frac{\mu(b_1^2 + b_2^2)}{8\pi(1-v)}\left[\frac{1}{2(1-v)} - \cos 2(\theta - \varphi)\right] \tag{23}$$

per unit length of the dislocation (Lubarda, 1997, 1998). The angle φ is defined by $\tan\varphi = b_2/b_1$, and the angle θ specifies the orientation of the cut surface across which the dislocation discontinuity is imposed (Fig. 4). The shear modulus and the Poisson's ratio of the medium are μ and v. In particular, for $\theta = \varphi$ and $\theta = \varphi + \pi/2$, (23) gives

$$\frac{1}{2}\int_{S^i} \widetilde{\mathbf{T}}^i \cdot \tilde{\mathbf{u}}^i\,\mathrm{d}S = \frac{\mu(b_1^2 + b_2^2)}{16\pi(1-v)^2} \cdot \begin{cases} (2v-1), & \theta = \varphi, \\ (3-2v), & \theta = \varphi + \frac{\pi}{2}. \end{cases} \tag{24}$$

These values are the minimum and maximum values that the work over the internal surface of the dislocation core can have for all straight cuts used to create the dislocation. Their difference is $\mu(b_1^2 + b_2^2)/4\pi(1-v)$, which can be interpreted as the work done by the net force over the core segment of the angle $\pi/2$ (from $\theta = \varphi$ to $\theta = \varphi + \pi/2$) on the translational displacements of amount b_1 and b_2, associated with the change of the displacement discontinuity from the cut surface $\theta = \varphi$ to $\theta = \varphi + \pi/2$. Note also that the core energy is the same if the displacement discontinuity of magnitude b is imposed at $\theta = \varphi$ or at $\theta = \varphi + \pi$, or if $b/2$ is imposed at $\theta = \varphi$ and $-b/2$ at $\theta = \varphi + \pi$.

The severe distortion of the material within the core region associated with the constant displacement discontinuity from the center of the core gives rise to singular stress and strain fields within the core, according to the linear elasticity theory. This divergence can be eliminated by using either non-linear or non-local elasticity models, or semi-discrete (quasicontinuum) models. The latter are based on atomistic models

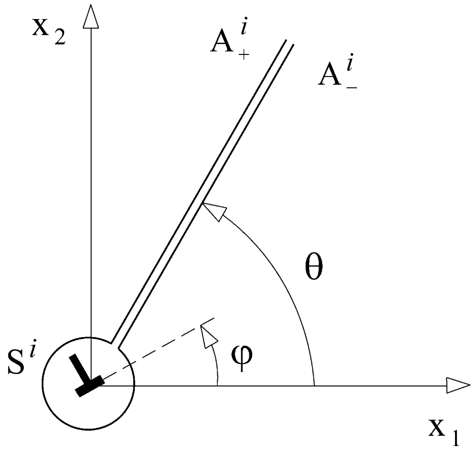

Fig. 4. Dislocation core around the straight dislocation with $b_2/b_1 = \tan\varphi$. The dislocation is created by imposing a displacement discontinuity $\mathbf{b} = \{b_1, b_2, b_3\}$ across the straight cut at an angle θ.

which take into account the crystallographic structure in the close proximity of the dislocation line, and the continuum elasticity description away from this region (Teodosiu, 1982; Tadmor et al., 1996). Hirth and Lothe (1982) report that atomistic calculations for glide dislocations in close-packed crystallographic structures suggest that the core energy per unit length of the dislocation is about $(0.05–0.1)\mu b^2$ (the core radius being of the order of b). The energy contribution given by the integral in (24) in the case of $\theta = \varphi$ is negative and equal to $-0.015\mu b^2$ (for $\nu = 1/3$). If the core energy per unit length of the straight dislocation is taken to be $\widetilde{U}^i_c = 0.075\mu b^2$, the misfit energy associated with the displacement discontinuity within the core, calculated from (22), is $0.06\mu b^2$ per unit length of the dislocation. This finite value of the core misfit energy corresponds to a gradual slip discontinuity within the core, embedded in a semi-discrete treatments of the core region. For example, if one adopts the Peierls–Nabarro dislocation model (Hirth and Lothe, 1982, p. 227), the misfit energy within the radius ρ, in its continuum approximation, is

$$W_\rho = \frac{\mu b^2}{4\pi^2(1-\nu)}\left[\ln\left(1+\frac{\rho^2}{\zeta^2}\right)\tan^{-1}\left(\frac{\rho}{\zeta}\right) - \int_0^{\rho/\zeta}\frac{\ln(1+z^2)}{1+z^2}\,\mathrm{d}z\right], \tag{25}$$

where $2\zeta = d/(1-\nu)$ and d is the atomic plane separation across the slip plane. The above integral can be evaluated numerically for any given ratio ρ/ζ. Formally, if $\rho \to R$, where R is a large cut-off radius, we obtain in the limit $R \gg \zeta$, $W_R = \mu b^2 \ln(R/2\zeta)/4\pi(1-\nu)$. If $\rho = \zeta$,

$$W_\zeta = \frac{\mu b^2}{4\pi^2(1-\nu)}\left(G - \frac{\pi}{4}\ln 2\right) = 0.09412\frac{\mu b^2}{1-\nu}, \tag{26}$$

where $G = 0.915965\ldots$ is Catalan's constant (Gradshteyn and Ryzhik, 1980). By taking $\rho = 1.8d$ as a more realistic value of the core radius, and $\nu = 1/3$, (25) gives $W_\rho = 0.06\mu b^2$.

Note that the total core energy $0.075\mu b^2$ is five times greater than the traction work $0.015\mu b^2$ over the external surface of the core (with the traction and displacement components at the core surface according to the Volterra dislocation model). The conclusion is that the second term in (5) is either infinite (idealized Volterra dislocation), or significantly greater than the first term (gradual slip discontinuity within the core). In either case, the expression (4) is an inadequate account of the total dislocation core energy. In the case of a screw dislocation, there are no stresses which do work on the cylindrical core surface (for the Volterra dislocation), so that the core energy is entirely due to slip discontinuity within the core. In the case of the Peierls–Nabarro dislocation model, this is given by (25) with omitted factor $(1 - \nu)$, and with

$\zeta = d/2$. If $\rho = 2d$, this misfit core energy is equal to $0.07\mu b^2$. These calculations are from the continuum model calculations; more realistic values of the core energy can be obtained by atomistic calculations which take into account the precise atomic rearrangement (disregistry) across the slip plane, and the corresponding interatomic force interactions (see, for example, Pasianot and Moreno-Gobbi (2004) and the references therein).

5. Dislocations in an externally loaded body

5.1. Mixed boundary conditions

Consider dislocation loops in a finite body of volume V under external traction $\mathbf{T}^{\rm ext}$ applied over the portion of the bounding surface S_T of the body. The displacement $\mathbf{u}^{\rm ext}$ is prescribed over the remaining part of the boundary $S_u = S - S_T$ (Fig. 5). The potential energy of the body and the loading system can be conveniently expressed as

$$\Pi = \frac{1}{2}\int_V (\boldsymbol{\sigma}_*^{\rm ext} + \boldsymbol{\sigma}^{\rm disl}) : (\boldsymbol{\epsilon}_*^{\rm ext} + \boldsymbol{\epsilon}^{\rm disl})\,\mathrm{d}V - \int_{S_T} \mathbf{T}^{\rm ext}\cdot(\mathbf{u}_*^{\rm ext} + \mathbf{u}^{\rm disl})\,\mathrm{d}S, \tag{27}$$

where $(\boldsymbol{\sigma}^{\rm disl}, \boldsymbol{\epsilon}^{\rm disl})$ are the stress and strain fields in an externally unloaded and unconstrained body due to dislocations alone ($\mathbf{T}^{\rm disl} = \mathbf{0}$ over S), while $(\boldsymbol{\sigma}_*^{\rm ext}, \boldsymbol{\epsilon}_*^{\rm ext})$ are the auxiliary stress and strain fields in a dislocation free body due to externally applied load $\mathbf{T}^{\rm ext}$ and adjusted displacement boundary conditions, such that

$$\begin{aligned} &\nabla\cdot\boldsymbol{\sigma}_*^{\rm ext} = \mathbf{0} \quad \text{in } V,\\ &\mathbf{n}\cdot\boldsymbol{\sigma}_*^{\rm ext} = \mathbf{T}^{\rm ext} \quad \text{on } S_T,\\ &\mathbf{u}_*^{\rm ext} = \mathbf{u}^{\rm ext} - \mathbf{u}^{\rm disl} \quad \text{on } S_u. \end{aligned} \tag{28}$$

The displacement field due to dislocations alone in an externally unloaded body is $\mathbf{u}^{\rm disl}$, so that $\mathbf{u}_*^{\rm ext} + \mathbf{u}^{\rm disl} = \mathbf{u}^{\rm ext}$ over S_u. The total stress and strain within the body are $\boldsymbol{\sigma} = \boldsymbol{\sigma}_*^{\rm ext} + \boldsymbol{\sigma}^{\rm disl}$ and $\boldsymbol{\epsilon} = \boldsymbol{\epsilon}_*^{\rm ext} + \boldsymbol{\epsilon}^{\rm disl}$, and the corresponding displacement is $\mathbf{u} = \mathbf{u}_*^{\rm ext} + \mathbf{u}^{\rm disl}$.

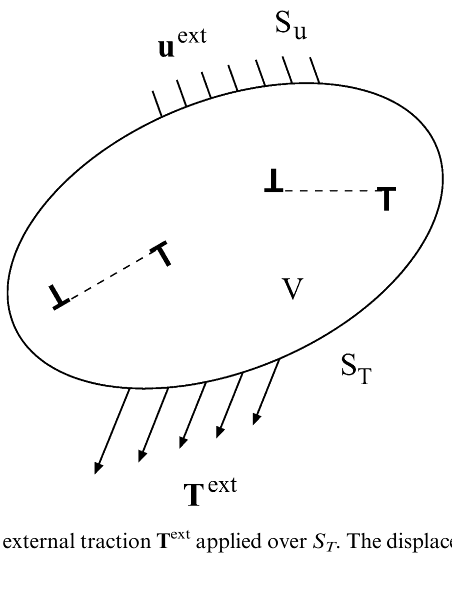

Fig. 5. Dislocations in a finite body under external traction $\mathbf{T}^{\rm ext}$ applied over S_T. The displacement $\mathbf{u}^{\rm ext}$ is prescribed over the remaining portion of the boundary S_u.

There is no cross-energy term between the externally applied stress and the internal self-equilibrating stress state, so that

$$\int_V \boldsymbol{\sigma}_*^{\text{ext}} : \boldsymbol{\epsilon}^{\text{disl}}\,\mathrm{d}V = \int_V \boldsymbol{\sigma}^{\text{disl}} : \boldsymbol{\epsilon}_*^{\text{ext}}\,\mathrm{d}V = \int_S \mathbf{T}^{\text{disl}} \cdot \mathbf{u}_*^{\text{ext}}\,\mathrm{d}S = 0. \tag{29}$$

The potential energy is consequently

$$\Pi = U^{\text{disl}} + \frac{1}{2}\int_V \boldsymbol{\sigma}_*^{\text{ext}} : \boldsymbol{\epsilon}_*^{\text{ext}}\,\mathrm{d}V - \int_{S_T} \mathbf{T}^{\text{ext}} \cdot (\mathbf{u}_*^{\text{ext}} + \mathbf{u}^{\text{disl}})\,\mathrm{d}S, \tag{30}$$

where U^{disl} is the strain energy of the body due to dislocations alone, as given by

$$U^{\text{disl}} = \frac{1}{2}\int_V \boldsymbol{\sigma}^{\text{disl}} : \boldsymbol{\epsilon}^{\text{disl}}\,\mathrm{d}V. \tag{31}$$

The simple structure of the potential energy expression (30) embeds the coupling between the external and dislocation stress and strain fields only implicitly, through the auxiliary fields $\boldsymbol{\sigma}_*^{\text{ext}}$ and $\boldsymbol{\epsilon}_*^{\text{ext}}$. Other representations of Π are also possible, e.g., Eshelby (1982), and Van der Giessen and Needleman (1995).

The variation of the potential energy Π, at fixed $\mathbf{T}^{\text{ext}}$ over S_T and fixed $\mathbf{u}^{\text{ext}}$ over S_u, is

$$\delta\Pi = \delta U^{\text{disl}} + \int_V \boldsymbol{\sigma}_*^{\text{ext}} : \delta\boldsymbol{\epsilon}_*^{\text{ext}}\,\mathrm{d}V - \int_S \mathbf{n}\cdot\boldsymbol{\sigma}_*^{\text{ext}} \cdot (\delta\mathbf{u}_*^{\text{ext}} + \delta\mathbf{u}^{\text{disl}})\,\mathrm{d}S. \tag{32}$$

The integration in the surface integral can be extended from S_T to S, because $\delta\mathbf{u}_*^{\text{ext}} + \delta\mathbf{u}^{\text{disl}} = \delta\mathbf{u}^{\text{ext}} = \mathbf{0}$ over S_u. Since

$$\int_V \boldsymbol{\sigma}_*^{\text{ext}} : \delta\boldsymbol{\epsilon}_*^{\text{ext}}\,\mathrm{d}V = \int_S \mathbf{n}\cdot\boldsymbol{\sigma}_*^{\text{ext}} \cdot \delta\mathbf{u}_*^{\text{ext}}\,\mathrm{d}S, \tag{33}$$

the variation of the potential energy becomes

$$\delta\Pi = \delta U^{\text{disl}} - \int_S \mathbf{n}\cdot\boldsymbol{\sigma}_*^{\text{ext}} \cdot \delta\mathbf{u}^{\text{disl}}\,\mathrm{d}S. \tag{34}$$

However, by the Gauss divergence theorem,

$$\int_V \boldsymbol{\sigma}_*^{\text{ext}} : \delta\boldsymbol{\epsilon}^{\text{disl}}\,\mathrm{d}V = \int_S \mathbf{n}\cdot\boldsymbol{\sigma}_*^{\text{ext}} \cdot \delta\mathbf{u}^{\text{disl}}\,\mathrm{d}S + \sum_{i=1}^{n}\int_{\delta A^i} \mathbf{n}^i\cdot\boldsymbol{\sigma}_*^{\text{ext}}\cdot\mathbf{b}^i\,\mathrm{d}(\delta A) \tag{35}$$

and since

$$\int_V \boldsymbol{\sigma}_*^{\text{ext}} : \delta\boldsymbol{\epsilon}^{\text{disl}}\,\mathrm{d}V = \int_V \delta\boldsymbol{\sigma}^{\text{disl}} : \boldsymbol{\epsilon}_*^{\text{ext}}\,\mathrm{d}V = \int_S \delta\mathbf{T}^{\text{disl}} \cdot \mathbf{u}_*^{\text{ext}}\,\mathrm{d}S = 0, \tag{36}$$

we deduce from (35) that

$$\int_S \mathbf{n}\cdot\boldsymbol{\sigma}_*^{\text{ext}} \cdot \delta\mathbf{u}^{\text{disl}}\,\mathrm{d}S = -\sum_{i=1}^{n}\int_{\delta A^i} \mathbf{n}^i\cdot\boldsymbol{\sigma}_*^{\text{ext}}\cdot\mathbf{b}^i\,\mathrm{d}(\delta A). \tag{37}$$

When this is substituted into (34), the variation of the potential energy becomes

$$\delta\Pi = \delta U^{\text{disl}} + \sum_{i=1}^{n}\int_{\delta A^i} \mathbf{n}^i\cdot\boldsymbol{\sigma}_*^{\text{ext}}\cdot\mathbf{b}^i\,\mathrm{d}(\delta A). \tag{38}$$

Finally, by incorporating (13) for δU^{disl}, there follows:

$$\delta\Pi = \sum_{i=1}^{n}\int_{\delta A^i} \mathbf{n}^i\cdot\left(\boldsymbol{\sigma}_*^{\text{ext}} + \hat{\boldsymbol{\sigma}} + \sum_{j\neq i}\tilde{\boldsymbol{\sigma}}^j\right)\cdot\mathbf{b}^i\,\mathrm{d}(\delta A). \tag{39}$$

The corresponding Peach–Koehler force along the dislocation line L^i is

$$\mathbf{f} = \mathbf{t} \times \left(\boldsymbol{\sigma}_*^{\text{ext}} + \hat{\boldsymbol{\sigma}} + \sum_{j \neq i} \tilde{\boldsymbol{\sigma}}^j \right) \cdot \mathbf{b}^i. \tag{40}$$

5.2. Traction boundary conditions

If the external traction $\mathbf{T}^{\text{ext}}$ is applied all over the bounding surface S of the body, the potential energy is

$$\Pi = \frac{1}{2} \int_V (\boldsymbol{\sigma}^{\text{ext}} + \boldsymbol{\sigma}^{\text{disl}}) : (\boldsymbol{\epsilon}^{\text{ext}} + \boldsymbol{\epsilon}^{\text{disl}})\, \mathrm{d}V - \int_S \mathbf{T}^{\text{ext}} \cdot (\mathbf{u}^{\text{ext}} + \mathbf{u}^{\text{disl}})\, \mathrm{d}S, \tag{41}$$

where $(\boldsymbol{\sigma}^{\text{ext}}, \boldsymbol{\epsilon}^{\text{ext}})$ are the stress and strain fields due to the externally applied load, defined such that

$$\begin{aligned} &\nabla \cdot \boldsymbol{\sigma}^{\text{ext}} = \mathbf{0} \quad \text{in } V, \\ &\mathbf{n} \cdot \boldsymbol{\sigma}^{\text{ext}} = \mathbf{T}^{\text{ext}} \quad \text{on } S. \end{aligned} \tag{42}$$

By following the analysis from the previous subsection, it readily follows that

$$\Pi = U^{\text{disl}} + \frac{1}{2} \int_V \boldsymbol{\sigma}^{\text{ext}} : \boldsymbol{\epsilon}^{\text{ext}}\, \mathrm{d}V - \int_{S_T} \mathbf{T}^{\text{ext}} \cdot (\mathbf{u}^{\text{ext}} + \mathbf{u}^{\text{disl}})\, \mathrm{d}S \tag{43}$$

and

$$\delta\Pi = \sum_{i=1}^{n} \int_{\delta A^i} \mathbf{n}^i \cdot \left(\boldsymbol{\sigma}^{\text{ext}} + \hat{\boldsymbol{\sigma}} + \sum_{j \neq i} \tilde{\boldsymbol{\sigma}}^j \right) \cdot \mathbf{b}^i\, \mathrm{d}(\delta A). \tag{44}$$

The Peach–Koehler force along the dislocation line L^i, due to the externally applied stress and the interaction of the dislocation with other dislocations and its own image field, is

$$\mathbf{f} = \mathbf{t} \times \left(\boldsymbol{\sigma}^{\text{ext}} + \hat{\boldsymbol{\sigma}} + \sum_{j \neq i} \tilde{\boldsymbol{\sigma}}^j \right) \cdot \mathbf{b}^i. \tag{45}$$

5.3. Displacement boundary conditions

If the dislocation loops are in the body with prescribed displacement $\mathbf{u}^{\text{ext}}$ over the whole boundary S, the potential energy is just the strain energy

$$\Pi = \frac{1}{2} \int_V (\boldsymbol{\sigma}_*^{\text{ext}} + \boldsymbol{\sigma}^{\text{disl}}) : (\boldsymbol{\epsilon}_*^{\text{ext}} + \boldsymbol{\epsilon}^{\text{disl}})\, \mathrm{d}V, \tag{46}$$

where $(\boldsymbol{\sigma}_*^{\text{ext}}, \boldsymbol{\epsilon}_*^{\text{ext}})$ are the stress and strain fields due to the adjusted displacement boundary conditions, such that

$$\begin{aligned} &\nabla \cdot \boldsymbol{\sigma}_*^{\text{ext}} = \mathbf{0} \quad \text{in } V, \\ &\mathbf{u}_*^{\text{ext}} = \mathbf{u}^{\text{ext}} - \mathbf{u}^{\text{disl}} \quad \text{on } S. \end{aligned} \tag{47}$$

The cross-energy term again vanishes, and the potential energy becomes

$$\Pi = U^{\text{disl}} + \frac{1}{2} \int_V \boldsymbol{\sigma}_*^{\text{ext}} : \boldsymbol{\epsilon}^{\text{ext}}\, \mathrm{d}V. \tag{48}$$

The variation of the potential energy Π, at fixed $\mathbf{u}^{\text{ext}}$ over S, is

$$\delta\Pi = \delta U^{\text{disl}} + \int_V \boldsymbol{\sigma}_*^{\text{ext}} : \delta\boldsymbol{\epsilon}_*^{\text{ext}}\,\mathrm{d}V. \tag{49}$$

Since $\delta\mathbf{u}^{\text{ext}} = \mathbf{0}$, i.e., $\delta\mathbf{u}_*^{\text{ext}} = -\delta\mathbf{u}^{\text{disl}}$, we have

$$\int_V \boldsymbol{\sigma}_*^{\text{ext}} : \delta\boldsymbol{\epsilon}_*^{\text{ext}}\,\mathrm{d}V = \int_S \mathbf{n}\cdot\boldsymbol{\sigma}_*^{\text{ext}}\cdot\delta\mathbf{u}_*^{\text{ext}}\,\mathrm{d}S = -\int_S \mathbf{n}\cdot\boldsymbol{\sigma}_*^{\text{ext}}\cdot\delta\mathbf{u}^{\text{disl}}\,\mathrm{d}S. \tag{50}$$

Consequently,

$$\delta\Pi = \delta U^{\text{disl}} - \int_S \mathbf{n}\cdot\boldsymbol{\sigma}_*^{\text{ext}}\cdot\delta\mathbf{u}^{\text{disl}}\,\mathrm{d}S. \tag{51}$$

The subsequent analysis proceeds as in Section 5.1, with the end result for the Peach–Koehler force according to (40).

6. Conclusions and discussion

We have derived in this paper the equilibrium conditions for a given collection of dislocations within a finite elastic body based on an energy expression that accounts for all of the dislocation core energy. This improves the previous derivation given in the literature which was based on an incomplete representation of the dislocation core energy. The difference between the two energy expressions is discussed in Section 4. For the dislocations with a fixed size and shape, the equilibrium conditions based on the two strain energy expressions (U and $\overline{U}$) are the same, because the variational principles $\delta U = 0$ and $\delta\overline{U} = 0$ impose the same conditions on the Peach–Koehler dislocation forces. This holds for the dislocations in an externally unloaded or loaded body, regardless of the type of the boundary conditions (Section 5). The reciprocity property of the misfit work, used in the derivation of the equilibrium conditions of Section 3, is proved in Appendix A of the paper.

The analysis presented in this paper was restricted to an idealized situation of the dislocations with a fixed size and shape. Furthermore, the interaction of the dislocation with itself was not considered. The latter is, of course, important for dislocation loops, since various segments of the loop interact among themselves. This gives rise to an additional force on an infinitesimal dislocation segment due to the stress state exerted there by other segments of the same dislocation. Gavazza and Barnett (1976) constructed a procedure to determine this self-force on a planar dislocation loop in an anisotropic infinite medium. If the loop is given a small perturbation in its shape ($\delta\mathbf{x}$ specified along L^i), the corresponding variation of the strain energy $\delta\widetilde{U}^i_{\text{self}}$ can be related to the configurational dislocation force $\tilde{\mathbf{f}}$ along the loop by

$$\delta\widetilde{U}^i_{\text{self}} = \int_{L^i} \tilde{\mathbf{f}}\cdot\delta\mathbf{x}\,\mathrm{d}L. \tag{52}$$

When dislocations are in a finite body, the dislocation loop will be in equilibrium if the dislocation force on each dislocation segment, due to its interaction with the remaining segments of the same dislocation and all other dislocations, as well as the externally applied stress, vanishes. Thus, for a body with mixed boundary conditions,

$$\mathbf{f} = \mathbf{t}\times\left(\boldsymbol{\sigma}_*^{\text{ext}} + \hat{\boldsymbol{\sigma}} + \sum_{j\neq i}\tilde{\boldsymbol{\sigma}}^j\right)\cdot\mathbf{b}^i + \tilde{\mathbf{f}} = \mathbf{0}, \tag{53}$$

at each point of the dislocation loop at its equilibrium configuration. If we consider the glide dislocations and include in the analysis the local lattice friction stress, representing a barrier for the outward and inward advance of the dislocation segment, the dislocation will be in equilibrium if, along the loop,

$$-f_{\text{glide}}^{-} \leqslant f_{\text{glide}} \leqslant f_{\text{glide}}^{+}, \quad f_{\text{glide}} = \mathbf{n}^i \cdot \left(\boldsymbol{\sigma}_*^{\text{ext}} + \hat{\boldsymbol{\sigma}} + \sum_{j \neq i} \tilde{\boldsymbol{\sigma}}^j \right) \cdot \mathbf{b}^i + \tilde{f}_{\text{glide}}. \tag{54}$$

While the determination of $\tilde{\mathbf{f}}$ is in general a difficult task, particularly for complicated dislocation geometries, its average value along the dislocation loop can in some cases be determined readily. For example, the mean tendency of the circular glide dislocation loop toward its self-similar shrinkage (annihilation) in an infinite isotropic medium is

$$\bar{f}_{\text{glide}} = -\frac{1}{2\pi R} \frac{\partial \widetilde{U}_{\text{self}}}{\partial R}, \tag{55}$$

where the current radius of the loop is R. The total self-energy of the circular dislocation, including the core energy and the energy outside the core region of radius $\rho \ll R$ (Hirth and Lothe, 1982), is

$$\widetilde{U}_{\text{self}} = 2\pi R \left[\frac{2-\nu}{1-\nu} \frac{\mu b^2}{8\pi} \left(\ln \frac{4R}{\rho} - 2 \right) + \alpha \mu b^2 \right]. \tag{56}$$

The term proportional to the parameter α accounts for the core energy. We assumed that the core energy of each infinitesimal segment of the loop is equal to that of a straight mixed-type dislocation tangent to the loop, so that α accounts for both edge and screw component contributions. If α is assumed to be constant (more generally, it could depend on R), from Eqs. (55) and (56) there follows

$$\bar{f}_{\text{glide}} = -\frac{\mu b^2}{R} \left[\frac{2-\nu}{1-\nu} \frac{1}{8\pi} \left(\ln \frac{4R}{\rho} - 1 \right) + \alpha \right]. \tag{57}$$

Gavazza and Barnett (1976) already calculated the shrinking tendency of the loop due to the change of the strain energy outside the toroidal core of the dislocation loop. LeSar (2004) recently examined different expressions for the self-energy of a dislocation loop, depending on the core cut-off procedure used to treat the severe material distortion in the vicinity of the dislocation line. Further research is needed, at both continuum and discrete–atomistic levels, to fully address the kinematics and kinetics of the dislocation core evolution during the expansion or annihilation of the dislocation loop. A significant insight can be gained from the related studies of mixed atomistic–continuum models of material behavior by Miller et al. (1998), Ortiz and Phillips (1999), and Ortiz et al. (2001).

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Appendix A. Reciprocal property of the misfit work

In the analysis of Section 3, by the Gauss divergence theorem we can write

$$\int_S \widehat{\mathbf{T}}^i \cdot \delta \tilde{\mathbf{u}}^i \, \mathrm{d}S + \int_{\delta A^i} \mathbf{n}^i \cdot \hat{\boldsymbol{\sigma}}^i \cdot \mathbf{b}^i \, \mathrm{d}(\delta A) = \int_V \hat{\boldsymbol{\sigma}}^i : \delta \tilde{\boldsymbol{\epsilon}}^i \, \mathrm{d}V, \tag{58}$$

and

$$\int_{\delta A^i} \mathbf{n}^i \cdot \boldsymbol{\sigma}^j \cdot \mathbf{b}^i \, \mathrm{d}(\delta A) = \int_V \boldsymbol{\sigma}^j : \delta \tilde{\boldsymbol{\epsilon}}^i \, \mathrm{d}V, \quad j \neq i, \quad \mathbf{T}^j = \mathbf{0} \quad \text{on } S. \tag{59}$$

The decompositions were used

$$\boldsymbol{\sigma}^i = \hat{\boldsymbol{\sigma}}^i + \tilde{\boldsymbol{\sigma}}^i, \quad \boldsymbol{\sigma} = \sum_{i=1}^n \boldsymbol{\sigma}^i, \quad \hat{\boldsymbol{\sigma}} = \sum_{i=1}^n \hat{\boldsymbol{\sigma}}^i. \tag{60}$$

By the summation of the previous expressions over $j \neq i$, we have

$$\int_S \widehat{\mathbf{T}}^i \cdot \delta\tilde{\mathbf{u}}^i \, \mathrm{d}S + \int_{\delta A^i} \mathbf{n}^i \cdot \left(\hat{\boldsymbol{\sigma}}^i + \sum_{j\neq i} \boldsymbol{\sigma}^j \right) \cdot \mathbf{b}^i \, \mathrm{d}(\delta A) = \int_V \left(\hat{\boldsymbol{\sigma}}^i + \sum_{j\neq i} \boldsymbol{\sigma}^j \right) : \delta\tilde{\boldsymbol{\epsilon}}^i \, \mathrm{d}V. \tag{61}$$

Similarly,

$$\int_S \widehat{\mathbf{T}}^i \cdot \tilde{\mathbf{u}}^i \, \mathrm{d}S + \int_{A^i} \mathbf{n}^i \cdot \left(\hat{\boldsymbol{\sigma}}^i + \sum_{j\neq i} \boldsymbol{\sigma}^j \right) \cdot \mathbf{b}^i \, \mathrm{d}A = \int_V \left(\hat{\boldsymbol{\sigma}}^i + \sum_{j\neq i} \boldsymbol{\sigma}^j \right) : \tilde{\boldsymbol{\epsilon}}^i \, \mathrm{d}V. \tag{62}$$

The variation of the sum of these expressions over i gives

$$\delta \sum_{i=1}^n \int_{A^i} \mathbf{n}^i \cdot \left(\hat{\boldsymbol{\sigma}}^i + \sum_{j\neq i} \boldsymbol{\sigma}^j \right) \cdot \mathbf{b}^i \, \mathrm{d}A = \delta \sum_{i=1}^n \int_V \left(\hat{\boldsymbol{\sigma}}^i + \sum_{j\neq i} \boldsymbol{\sigma}^j \right) : \tilde{\boldsymbol{\epsilon}}^i \, \mathrm{d}V - \delta \sum_{i=1}^n \int_S \widehat{\mathbf{T}}^i \cdot \tilde{\mathbf{u}}^i \, \mathrm{d}S. \tag{63}$$

Next we show that

$$\delta \sum_{i=1}^n \int_V \left(\hat{\boldsymbol{\sigma}}^i + \sum_{j\neq i} \boldsymbol{\sigma}^j \right) : \tilde{\boldsymbol{\epsilon}}^i \, \mathrm{d}V = 2 \sum_{i=1}^n \int_V \left(\hat{\boldsymbol{\sigma}}^i + \sum_{j\neq i} \boldsymbol{\sigma}^j \right) : \delta\tilde{\boldsymbol{\epsilon}}^i \, \mathrm{d}V. \tag{64}$$

First, since

$$\hat{\boldsymbol{\sigma}}^i + \sum_{j\neq i} \boldsymbol{\sigma}^j = \hat{\boldsymbol{\sigma}} + \sum_{j\neq i} \tilde{\boldsymbol{\sigma}}^j, \tag{65}$$

the previous expression can be rewritten as

$$\delta \sum_{i=1}^n \int_V \left(\hat{\boldsymbol{\sigma}} + \sum_{j\neq i} \tilde{\boldsymbol{\sigma}}^j \right) : \tilde{\boldsymbol{\epsilon}}^i \, \mathrm{d}V = 2 \sum_{i=1}^n \int_V \left(\hat{\boldsymbol{\sigma}} + \sum_{j\neq i} \tilde{\boldsymbol{\sigma}}^j \right) : \delta\tilde{\boldsymbol{\epsilon}}^i \, \mathrm{d}V. \tag{66}$$

Then,

$$\delta \sum_{i=1}^n \sum_{j\neq i} \int_V \tilde{\boldsymbol{\sigma}}^j : \tilde{\boldsymbol{\epsilon}}^i \, \mathrm{d}V = 2 \sum_{i=1}^n \sum_{j\neq i} \int_V \tilde{\boldsymbol{\sigma}}^j : \delta\tilde{\boldsymbol{\epsilon}}^i \, \mathrm{d}V, \tag{67}$$

and

$$\int_V \hat{\boldsymbol{\sigma}} : \sum_{i=1}^n \tilde{\boldsymbol{\epsilon}}^i \, \mathrm{d}V = \int_V \sum_{i=1}^n \tilde{\boldsymbol{\sigma}}^i : \hat{\boldsymbol{\epsilon}} \, \mathrm{d}V = \int_S \sum_{i=1}^n \widetilde{\mathbf{T}}^i \cdot \hat{\mathbf{u}} \, \mathrm{d}S = -\int_S \widehat{\mathbf{T}} \cdot \hat{\mathbf{u}} \, \mathrm{d}S = -\int_V \hat{\boldsymbol{\sigma}} : \hat{\boldsymbol{\epsilon}} \, \mathrm{d}V. \tag{68}$$

The variation of the above integral is

$$\begin{aligned} \delta \int_V \hat{\boldsymbol{\sigma}} : \sum_{i=1}^n \tilde{\boldsymbol{\epsilon}}^i \, \mathrm{d}V &= -2 \int_V \delta\hat{\boldsymbol{\sigma}} : \hat{\boldsymbol{\epsilon}} \, \mathrm{d}V = -2 \int_S \delta\widehat{\mathbf{T}} \cdot \hat{\mathbf{u}} \, \mathrm{d}S = 2 \int_S \sum_{i=1}^n \delta\widetilde{\mathbf{T}}^i \cdot \hat{\mathbf{u}} \, \mathrm{d}S \\ &= 2 \int_V \sum_{i=1}^n \delta\tilde{\boldsymbol{\sigma}}^i : \hat{\boldsymbol{\epsilon}} \, \mathrm{d}V = 2 \int_V \hat{\boldsymbol{\sigma}} : \sum_{i=1}^n \delta\tilde{\boldsymbol{\epsilon}}^i \, \mathrm{d}V. \end{aligned}$$

The substitution of this expression and (67) into (66) proves the equality.

Consider now an infinite medium with the extracted volume V and dislocations with it. The internal surface S of the hollow medium $V_\infty - V$ is under the traction fields $\widehat{\mathbf{T}}^i = -\widetilde{\mathbf{T}}^i$ and the corresponding displacement fields $\tilde{\mathbf{u}}^i$ from each dislocation. For every pair of these we can write by the Gauss divergence theorem

$$\int_S \widehat{\mathbf{T}}^i \cdot \tilde{\mathbf{u}}^i \,\mathrm{d}S = \int_{V_\infty - V} \tilde{\boldsymbol{\sigma}}^i : \tilde{\boldsymbol{\epsilon}}^i \,\mathrm{d}V. \tag{69}$$

Thus,

$$\delta \int_S \widehat{\mathbf{T}}^i \cdot \tilde{\mathbf{u}}^i \,\mathrm{d}S = 2 \int_S \widehat{\mathbf{T}}^i \cdot \delta\tilde{\mathbf{u}}^i \,\mathrm{d}S, \tag{70}$$

because $\delta\tilde{\boldsymbol{\sigma}}^i : \tilde{\epsilon}^i = \tilde{\boldsymbol{\sigma}}^i : \delta\tilde{\epsilon}^i$ by the reciprocal symmetry of the elastic moduli tensor and by the symmetry of the stress and strain tensors. When (64) and (70) are substituted into (63), there follows:

$$\delta \sum_{i=1}^{n} \int_{A^i} \mathbf{n}^i \cdot \left(\hat{\boldsymbol{\sigma}}^i + \sum_{j\neq i} \boldsymbol{\sigma}^j \right) \cdot \mathbf{b}^i \,\mathrm{d}A = 2 \sum_{i=1}^{n} \int_V \left(\hat{\boldsymbol{\sigma}}^i + \sum_{j\neq i} \boldsymbol{\sigma}^j \right) : \delta\tilde{\epsilon}^i \,\mathrm{d}V - 2 \sum_{i=1}^{n} \int_S \widehat{\mathbf{T}}^i \cdot \delta\tilde{\mathbf{u}}^i \,\mathrm{d}S. \tag{71}$$

The comparison with (61), summed over i, shows that

$$\delta \sum_{i=1}^{n} \int_{A^i} \mathbf{n}^i \cdot \left(\hat{\boldsymbol{\sigma}}^i + \sum_{j\neq i} \boldsymbol{\sigma}^j \right) \cdot \mathbf{b}^i \,\mathrm{d}A = 2 \sum_{i=1}^{n} \int_{\delta A^i} \mathbf{n}^i \cdot \left(\hat{\boldsymbol{\sigma}}^i + \sum_{j\neq i} \boldsymbol{\sigma}^j \right) \cdot \mathbf{b}^i \,\mathrm{d}(\delta A). \tag{72}$$

Invoking (65) again we establish the reciprocal property of the misfit work,

$$\sum_{i=1}^{n} \int_{A^i} \mathbf{n}^i \cdot \left(\delta\hat{\boldsymbol{\sigma}} + \sum_{j\neq i} \delta\tilde{\boldsymbol{\sigma}}^j \right) \cdot \mathbf{b}^i \,\mathrm{d}A = \sum_{i=1}^{n} \int_{\delta A^i} \mathbf{n}^i \cdot \left(\hat{\boldsymbol{\sigma}} + \sum_{j\neq i} \tilde{\boldsymbol{\sigma}}^j \right) \cdot \mathbf{b}^i \,\mathrm{d}(\delta A), \tag{73}$$

which was used in arriving at Eq. (14) of Section 3.

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