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On the elastic strain energy representation of a dislocated body and dislocation equilibrium conditions

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Abstract. Various equilibrium dislocation distributions in finite and infinite media were recently analyzed [5], both from theoretical and computational standpoints. In this paper we shed further light on this issue, by elaborating on a variational procedure that gives the required equilibrium conditions: the glide forces on each dislocation represent a set of self-equilibrating forces. The derivation is carried out in a general 3-dimensional setting, with adequate specifications for edge dislocations in plain-strain case.

1. Introduction

Two alternative superposition procedures are introduced to define the stress and strain fields in a dislocated body and to obtain the corresponding, simple representations of the elastic strain energy. The associated variational expressions are then derived, which give from the stationary energy requirement the required dislocation equilibrium conditions. Dislocations are assumed to be of fixed type and geometry, so that during variation they can move along their slip planes only as rigid entities. In the analysis that follows, two theorems were extensively utilized, i.e. the Gauss divergence and the well-known linear elasticity theorem [3, 8]:

"In the expression for the total elastic strain energy of a stressed body, there is no cross term between the internal stress (locked-in stresses present when no external forces act) and the stress caused by externally applied forces." (Theorem 1)

Indeed, let finite or infinite body V be in the state of initial stress ($\boldsymbol{\sigma}^0$) and strain ($\boldsymbol{\varepsilon}^0$) distributions, such as those resulting from the presence of dislocation imperfections within the body (a dislocated body). The corresponding (initial) elastic strain energy is

$$U_V^0 = \frac{1}{2}\int_V \boldsymbol{\sigma}^0 : \boldsymbol{\varepsilon}^0 \, \mathrm{d}V, \tag{1.1}$$

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where : denotes the trace. Apply the surface traction $\mathbf{t}^*$ over the external (or imagined internal) surface on such a body, and let $\boldsymbol{\sigma}^*$ and $\boldsymbol{\varepsilon}^*$ be the corresponding stress and strain fields which would be determined from the elasticity solution if there were no dislocations within the body. The additional strain energy stored in the dislocated body is

$$\frac{1}{2}\int_V \boldsymbol{\sigma}^*:\boldsymbol{\varepsilon}^*\,\mathrm{d}V + \int_V \boldsymbol{\sigma}^0:\boldsymbol{\varepsilon}^*\,\mathrm{d}V,$$

(provided that internal stresses are locked-in, i.e. that dislocations do not move when applying $\mathbf{t}^*$). The second term, which represents the work done by the already existing stress $\boldsymbol{\sigma}^0$ on additional strain $\boldsymbol{\varepsilon}^*$, is, however, equal to zero, since equilibrium and the Gauss divergence theorem show

$$\int_V \boldsymbol{\sigma}^0:\boldsymbol{\varepsilon}^*\,\mathrm{d}V = \int_S \mathbf{t}^0\cdot\mathbf{u}^*\,\mathrm{d}S = 0, \tag{1.2}$$

and the bounding surface S of the body V in its initial dislocated configuration is traction free ($\mathbf{t}^0 = \mathbf{0}$). Therefore, the total strain energy of the body is simply

$$U_V^T = \frac{1}{2}\int_V \boldsymbol{\sigma}^0:\boldsymbol{\varepsilon}^0\,\mathrm{d}V + \frac{1}{2}\int_V \boldsymbol{\sigma}^*:\boldsymbol{\varepsilon}^*\,\mathrm{d}V, \tag{1.3}$$

without the energy cross-term contribution from the two different fields. The superposition principle of linear elasticity reveals that total stress and strain are $(\boldsymbol{\sigma}^0 + \boldsymbol{\sigma}^*)$ and $(\boldsymbol{\varepsilon}^0 + \boldsymbol{\varepsilon}^*)$. The strain energy can also be written as

$$U_V^T = \frac{1}{2}\int_V (\boldsymbol{\sigma}^0 + \boldsymbol{\sigma}^*):(\boldsymbol{\varepsilon}^0 + \boldsymbol{\varepsilon}^*)\,\mathrm{d}V \tag{1.4}$$

and by incorporating (1.2) and (1.3), we have in addition

$$\int_V \boldsymbol{\sigma}^*:\boldsymbol{\varepsilon}^0\,\mathrm{d}V = 0. \tag{1.5}$$

This equation can also follow directly from (1.2) by applying the generalized Hooke's law which gives $\boldsymbol{\sigma}^0 = \mathbf{L}:\boldsymbol{\varepsilon}^0$ and $\boldsymbol{\sigma}^* = \mathbf{L}:\boldsymbol{\varepsilon}^*$, where $\mathbf{L}$ denotes the tensor of elastic moduli.

The results above are often called upon in the following sections, where we elaborate on the initial strain energy expression for the dislocated finite body by introducing an adequate superposition procedure to evaluate the stress and strain fields, $\boldsymbol{\sigma}^0$ and $\boldsymbol{\varepsilon}^0$. In dislocation theory, superposition is usually defined with respect to infinite medium dislocation solutions, since these are often available or can be determined more readily [1, 3, 4].

2. The strain energy of a dislocated body

Consider the body of finite volume V bounded by surface S which contains a given number of dislocations. Let the external surface S be traction free, so that the stress field $\boldsymbol{\sigma}$ comes only from the dislocations within the body. If $\boldsymbol{\varepsilon}$ is the corresponding elastic strain, the strain energy is

$$U_V = \frac{1}{2}\int_V \boldsymbol{\sigma} : \boldsymbol{\varepsilon} \, dV \tag{2.1}$$

(for the simplicity of notation, the superimposed o which indicates initial is henceforth omitted). Since $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$ are singular at the points of dislocation lines, we can suppose that U_V is prevented from diverging by omitting the interior of the small-radius tubes embracing the singular lines (dislocation core energies) from the integration, [1], or alternatively by using the scheme from [5], where the core energies were represented by certain nonvanishing surface integrals. We further elaborate on expression (2.1) by introducing an adequate superposition procedure to define the required stress and strain fields, and thus obtain the corresponding strain energy representation.

2.1. *The strain energy representation*

Consider dislocations from body V to be submerged (in the same relative configuration) in an infinite medium, and denote the corresponding stress field by $\tilde{\boldsymbol{\sigma}}$. Introduce an auxiliary problem in which a dislocation free infinite medium is loaded over the internal surface S, coinciding with the bounding surface of V, by traction $\bar{\mathbf{t}}$, which sets up the stress field $\bar{\boldsymbol{\sigma}}$ such that, on superimposing two solutions, we have within the volume V: $\tilde{\boldsymbol{\sigma}} + \bar{\boldsymbol{\sigma}} = \boldsymbol{\sigma}$ (Fig. 1). The strain energy of the resulting, dislocated infinite medium, loaded by traction $\bar{\mathbf{t}}$, is simply the sum of the strain energies due to dislocations and traction alone, $U_\infty = \tilde{U}_\infty + \bar{U}_\infty$, i.e.

$$U_\infty = \frac{1}{2}\int_\infty \tilde{\boldsymbol{\sigma}} : \tilde{\boldsymbol{\varepsilon}} \, dV + \frac{1}{2}\int_S \bar{\mathbf{t}} \cdot \bar{\mathbf{u}} \, dS. \tag{2.2}$$

Here $\tilde{\boldsymbol{\varepsilon}}$ is the infinite medium dislocation strain field and $\bar{\mathbf{u}}$ displacement on S due to traction $\bar{\mathbf{t}}$ in the undislocated infinite medium. As discussed in the

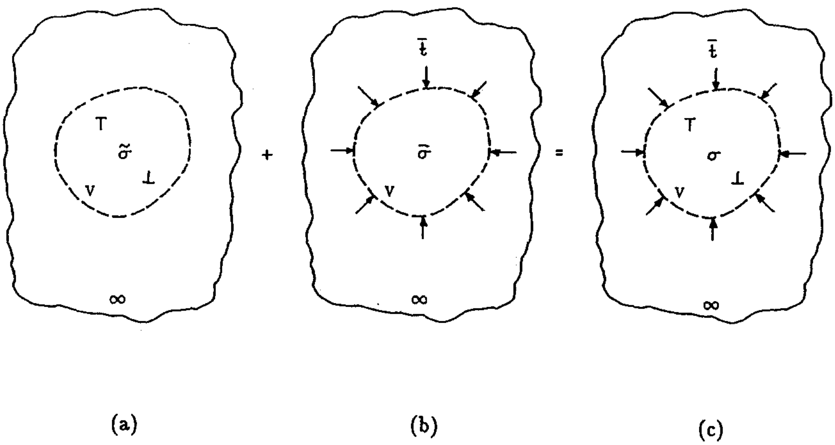


Fig. 1. Superposition of: (a) dislocated infinite medium, and (b) undislocated infinite medium loaded by traction $\bar{\mathbf{t}}$; the stress and strain distributions within V of the resulting configuration (c) are those of the traction-free dislocated body V.

Introduction, by Theorem 1 there is no energy cross-term resulting from the interaction of two different fields. But, the stress distribution $\boldsymbol{\sigma}$ within the volume V does not give rise to any traction $\mathbf{t}$ on the bounding surface S, hence the volume V on Fig. 1c can be taken out from the infinite medium, such that all traction $\bar{\mathbf{t}}$ acts on the surface S bounding the hole in the remaining part of (dislocation free) infinite body. The strain energy can, consequently, be also expressed as

$$U_\infty = U_V + \frac{1}{2}\int_S \bar{\mathbf{t}}\cdot\mathbf{u}\,\mathrm{d}S, \tag{2.3}$$

with $\mathbf{u}$ being displacement field on the surface S. Note that the surface integral on the right-hand side of (2.3) is, by Gauss's theorem, the strain energy $U_{(\infty - V)} = \frac{1}{2}\int_{(\infty - V)} \boldsymbol{\sigma}:\boldsymbol{\varepsilon}\,\mathrm{d}V$. Equating (2.2) and (2.3), we then obtain the following expression for the strain energy of the traction-free dislocated body

$$U_V = \frac{1}{2}\int_\infty \tilde{\boldsymbol{\sigma}}:\tilde{\boldsymbol{\varepsilon}}\,\mathrm{d}V - \frac{1}{2}\int_S \bar{\mathbf{t}}\cdot\tilde{\mathbf{u}}\,\mathrm{d}S, \tag{2.4}$$

where $\tilde{\mathbf{u}} = \mathbf{u} - \bar{\mathbf{u}}$ is the displacement over S caused by dislocations in the infinite medium.

2.2. *An alternative representation*

We now derive an alternative expression for U_V by considering, as in [5], the stress and strain fields $(\boldsymbol{\sigma}, \boldsymbol{\varepsilon})$ of the dislocated body V to be obtained by superposition of the infinite medium dislocation fields $(\tilde{\boldsymbol{\sigma}}, \tilde{\boldsymbol{\varepsilon}})$ and $(\hat{\boldsymbol{\sigma}}, \hat{\boldsymbol{\varepsilon}})$ fields resulting from the traction $\hat{\mathbf{t}} = -\tilde{\mathbf{t}}$ which is applied on the surface S of the auxiliary, dislocation free body V (Fig. 2). Here, $\tilde{\mathbf{t}}$ is the traction set up on the surface S by dislocations in the infinite medium, which needs to be canceled by the traction $\hat{\mathbf{t}}$ of the auxiliary problem in order to obtain the traction free boundary condition of the condition of the dislocated body V. Hence, since $\boldsymbol{\sigma} = \tilde{\boldsymbol{\sigma}} + \hat{\boldsymbol{\sigma}}$ and $\boldsymbol{\varepsilon} = \tilde{\boldsymbol{\varepsilon}} + \hat{\boldsymbol{\varepsilon}}$, the strain energy is

$$U_V = \frac{1}{2}\int_V \tilde{\boldsymbol{\sigma}}:\tilde{\boldsymbol{\varepsilon}}\,\mathrm{d}V + \frac{1}{2}\int_V \hat{\boldsymbol{\sigma}}:\hat{\boldsymbol{\varepsilon}}\,\mathrm{d}V + \frac{1}{2}\left(\int_V \tilde{\boldsymbol{\sigma}}:\hat{\boldsymbol{\varepsilon}}\,\mathrm{d}V + \int_V \hat{\boldsymbol{\sigma}}:\tilde{\boldsymbol{\varepsilon}}\,\mathrm{d}V\right). \tag{2.5}$$

But, by the Theorem 1 we have

$$\int_V \boldsymbol{\sigma}:\hat{\boldsymbol{\varepsilon}}\,\mathrm{d}V = 0 \quad \text{and} \quad \int_V \hat{\boldsymbol{\sigma}}:\boldsymbol{\varepsilon}\,\mathrm{d}V = 0, \tag{2.6}$$

so that the reciprocal relation holds,

$$\int_V \tilde{\boldsymbol{\sigma}}:\hat{\boldsymbol{\varepsilon}}\,\mathrm{d}V = \int_V \hat{\boldsymbol{\sigma}}:\tilde{\boldsymbol{\varepsilon}}\,\mathrm{d}V\left(= -\int_V \hat{\boldsymbol{\sigma}}:\hat{\boldsymbol{\varepsilon}}\,\mathrm{d}V\right), \tag{2.7}$$

which, of course, also follows from the generalized Hooke's law which gives $\tilde{\boldsymbol{\sigma}} = \mathbf{L}:\tilde{\boldsymbol{\varepsilon}}$ and $\hat{\boldsymbol{\sigma}} = \mathbf{L}:\hat{\boldsymbol{\varepsilon}}$. Substituting (2.7) into (2.5), we then have

$$U_V = \frac{1}{2}\int_V \tilde{\boldsymbol{\sigma}}:\tilde{\boldsymbol{\varepsilon}}\,\mathrm{d}V - \frac{1}{2}\int_S \hat{\mathbf{t}}\cdot\hat{\mathbf{u}}\,\mathrm{d}S, \tag{2.8}$$

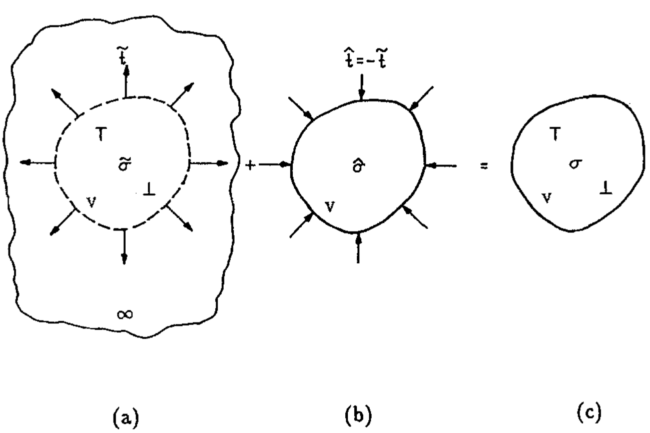


Fig. 2. Superposition of: (a) dislocated infinite medium, and (b) undislocated finite body V loaded by traction $\hat{\mathbf{t}} = -\tilde{\mathbf{t}}$, to obtain solution (c) of the traction-free dislocated body V.

utilizing $\int_V \hat{\boldsymbol{\sigma}}:\hat{\boldsymbol{\varepsilon}}\,\mathrm{d}V = \int_S \hat{\mathbf{t}}\cdot\hat{\mathbf{u}}\,\mathrm{d}S$. The volume integral on the right-hand side of (2.8) is the portion of the infinite medium dislocation energy contained within the volume V ($\tilde{U}_V$), which can be related to $\tilde{U}_\infty$ by

$$\tilde{U}_\infty = \frac{1}{2}\int_\infty \tilde{\boldsymbol{\sigma}}:\tilde{\boldsymbol{\varepsilon}}\,\mathrm{d}V = \frac{1}{2}\int_V \tilde{\boldsymbol{\sigma}}:\tilde{\boldsymbol{\varepsilon}}\,\mathrm{d}V + \frac{1}{2}\int_S \hat{\mathbf{t}}\cdot\tilde{\mathbf{u}}\,\mathrm{d}S. \tag{2.9}$$

The surface integral in (2.9) is obtained by applying the Gauss theorem to the dislocation free ($\infty - V$) portion of the infinite medium obtained by taking out the dislocated volume V (Fig. 2a); the surface of the hole is under the traction $\hat{\mathbf{t}} = -\bar{\mathbf{t}}$, and by Gauss's theorem

$$\int_{(\infty - V)} \tilde{\sigma}:\tilde{\boldsymbol{\varepsilon}}\,\mathrm{d}V = \int_S \hat{\mathbf{t}}\cdot\tilde{\mathbf{u}}\,\mathrm{d}S. \tag{2.10}$$

Substitution of (2.9) into (2.8) therefore gives

$$U_V = \frac{1}{2}\int_\infty \tilde{\boldsymbol{\sigma}}:\tilde{\boldsymbol{\varepsilon}}\,\mathrm{d}V - \frac{1}{2}\int_S \hat{\mathbf{t}}\cdot\mathbf{u}\,\mathrm{d}S, \tag{2.11}$$

where $\mathbf{u} = \tilde{\mathbf{u}} + \hat{\mathbf{u}}$ is the displacement over the boundary S of the dislocated body V, measured from its undislocated (stress and strain free) initial configuration.

2.3. *The equivalence demonstration*

The two obtained expressions for the strain energy, (2.4) and (2.11), are of course equivalent, as the identity which is formally shown in this subsection,

$$\int_S \bar{\mathbf{t}}\cdot\tilde{\mathbf{u}}\,\mathrm{d}S = \int_S \hat{\mathbf{t}}\cdot\mathbf{u}\,\mathrm{d}S, \tag{2.12}$$

must hold. We start with the obvious equality

$$\int_S \bar{\mathbf{t}}\cdot\tilde{\mathbf{u}}\,\mathrm{d}S = \int_S (\bar{\mathbf{t}} + \hat{\mathbf{t}})\cdot\tilde{\mathbf{u}}\,\mathrm{d}S - \int_S \hat{\mathbf{t}}\cdot\tilde{\mathbf{u}}\,\mathrm{d}S. \tag{2.13}$$

The physical meaning of the traction ($\bar{\mathbf{t}} + \hat{\mathbf{t}}$) is illustrated in Fig. 3, which shows the superposition of two solutions that give the dislocation free infinite body loaded by traction $\bar{\mathbf{t}}$ over the internal surface S, as previously introduced in Fig.

1b. As in the $(\infty - V)$ portion of the body in Fig. 1a, the displacement $\tilde{\mathbf{u}}$ is continuous, the Gauss formula gives

$$\int_{(\infty - V)} \bar{\boldsymbol{\sigma}}:\tilde{\boldsymbol{\varepsilon}}\,\mathrm{d}V = \int_S (\bar{\mathbf{t}} + \tilde{\mathbf{t}})\cdot\tilde{\mathbf{u}}\,\mathrm{d}S. \tag{2.14}$$

Since by Theorem 1 we have $\int_\infty \bar{\boldsymbol{\sigma}}:\tilde{\boldsymbol{\varepsilon}}\,\mathrm{d}V = 0$, (2.13) becomes

$$\int_S \bar{\mathbf{t}}\cdot\tilde{\mathbf{u}}\,\mathrm{d}S = -\int_V \bar{\boldsymbol{\sigma}}:\tilde{\boldsymbol{\varepsilon}}\,\mathrm{d}V - \int_S \tilde{\mathbf{t}}\cdot\tilde{\mathbf{u}}\,\mathrm{d}S. \tag{2.15}$$

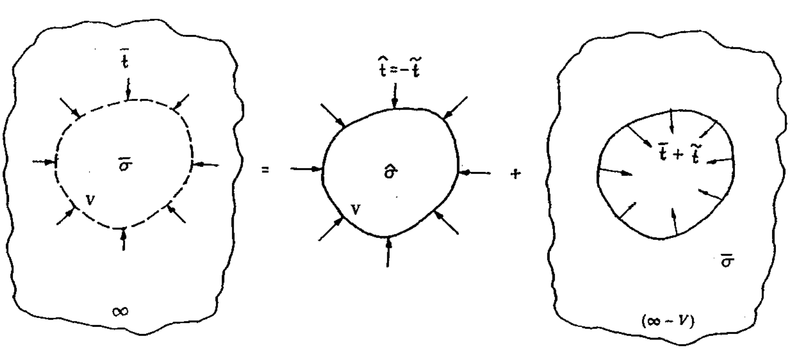
But, within the volume V, $\bar{\boldsymbol{\sigma}} \equiv \hat{\boldsymbol{\sigma}}$, hence by the reciprocity and Gauss theorems

$$\int_V \hat{\boldsymbol{\sigma}}:\tilde{\boldsymbol{\varepsilon}}\,\mathrm{d}V = \int_V \tilde{\boldsymbol{\sigma}}:\hat{\boldsymbol{\varepsilon}}\,\mathrm{d}V = \int_S \tilde{\mathbf{t}}\cdot\hat{\mathbf{u}}\,\mathrm{d}S, \tag{2.16}$$

and substitution into (2.15) establishes the identity (2.12).

Note that the superposition sketched in Fig. 3 also gives the condition for explicit determination of the traction $\tilde{\mathbf{t}}$: displacements over the surface S on Figs. 3b and 3c must be the same, i.e.

$$\bar{\mathbf{u}}^{\hat{t}}_{S_V} = \bar{\mathbf{u}}^{\bar{t}+\tilde{t}}_{S_{(\infty - V)}}. \tag{2.17}$$



(a) (b) (c)

Fig. 3. Undislocated infinite medium (a) loaded by traction $\bar{\mathbf{t}}$, as a superposition of: (b) finite body V loaded by traction $\hat{\mathbf{t}} = -\tilde{\mathbf{t}}$, and (c) the remaining $(\infty - V)$ body loaded by traction $\bar{\mathbf{t}} + \tilde{\mathbf{t}}$ over the hole surface.

However, to determine the stress and strain distributions $\hat{\boldsymbol{\sigma}}$ and $\hat{\boldsymbol{\varepsilon}}$, it is easier to solve the auxiliary problem with the traction $\hat{\mathbf{t}}$ on the surface S of V. An explicit evaluation of $\hat{\mathbf{t}}$ is, in fact, not needed. Its significance is in the simplicity that results in the derivation leading to the equilibrium conditions for the dislocation distribution, as discussed in the body of the paper.

3. Expressions involving dislocation slip

Consider again the configuration in Fig. 1c, i.e. the infinite medium which contains dislocations within the volume V and which is loaded by traction $\bar{\mathbf{t}}$ over the surface S. This configuration can be imagined to be obtained in two alternative sequences. First, introduce dislocations into the undislocated infinite medium, and then apply the traction $\bar{\mathbf{t}}$. The strain energy of the final state is by Theorem 1

$$U_\infty = \frac{1}{2}\int_\infty \tilde{\boldsymbol{\sigma}}:\tilde{\boldsymbol{\varepsilon}}\,\mathrm{d}V + \frac{1}{2}\int_S \bar{\mathbf{t}}\cdot\bar{\mathbf{u}}\,\mathrm{d}S. \tag{3.1}$$

Obtain now the final state in the reverse order, i.e. first apply $\bar{\mathbf{t}}$, and then introduce dislocations; the strain energy is

$$U_\infty = \frac{1}{2}\int_S \bar{\mathbf{t}}\cdot\bar{\mathbf{u}}\,\mathrm{d}S + \frac{1}{2}\int_\infty \tilde{\boldsymbol{\sigma}}:\tilde{\boldsymbol{\varepsilon}}\,\mathrm{d}V + \int_S \bar{\mathbf{t}}\cdot\tilde{\mathbf{u}}\,\mathrm{d}S - \sum_{\text{disl}}\int_{A_{\text{slip}}} (\mathbf{n}\cdot\hat{\boldsymbol{\sigma}}\cdot\mathbf{b})\,\mathrm{d}A_{\text{slip}}. \tag{3.2}$$

The third integral on the right-hand side of (3.2) is the work done by the already existing traction $\bar{\mathbf{t}}$ on displacement $\tilde{\mathbf{u}}$ of S, which is caused by the introduction of dislocations. The last term is carried out by traction $\bar{\mathbf{t}}_{-n} = -\mathbf{n}\cdot\hat{\boldsymbol{\sigma}}$, which acts over the areas within the dislocation loops A_{slip} on the (discontinuous) slip displacements of the amount $\mathbf{b}$, the Burgers vector ($\mathbf{n}$ stands for the normal to A_{slip}, so that the material above A_{slip} is slipped in the direction of $\mathbf{b}$; note also that within V: $\bar{\boldsymbol{\sigma}} \equiv \hat{\boldsymbol{\sigma}}$). Therefore, since in linear elasticity the order in which we load the body does not influence the final state, (3.2) is the same as (3.1), and therefore

$$\int_S \bar{\mathbf{t}}\cdot\tilde{\mathbf{u}}\,\mathrm{d}S = \sum_{\text{disl}}\int_{A_{\text{slip}}} (\mathbf{n}\cdot\hat{\boldsymbol{\sigma}}\cdot\mathbf{b})\,\mathrm{d}A_{\text{slip}}. \tag{3.3}$$

This also can be deduced by applying the Gauss theorem to the following integral

$$\int_{\infty} \bar{\boldsymbol{\sigma}}:\tilde{\boldsymbol{\varepsilon}}\,\mathrm{d}V = \int_{S} \bar{\mathbf{t}}\cdot\tilde{\mathbf{u}}\,\mathrm{d}S - \sum_{\text{disl}} \int_{A_{\text{slip}}} (\mathbf{n}\cdot\hat{\boldsymbol{\sigma}}\cdot\mathbf{b})\,\mathrm{d}A_{\text{slip}}, \tag{3.4}$$

which by Theorem 1 is equal to zero. Hence, we again obtain (3.3). Similarly, the Gauss theorem gives

$$\int_{V} \hat{\boldsymbol{\sigma}}:\boldsymbol{\varepsilon}\,\mathrm{d}V = \int_{S} \hat{\mathbf{t}}\cdot\mathbf{u}\,\mathrm{d}S - \sum_{\text{disl}} \int_{A_{\text{slip}}} (\mathbf{n}\cdot\hat{\boldsymbol{\sigma}}\cdot\mathbf{b})\,\mathrm{d}A_{\text{slip}}; \tag{3.5}$$

and since by Theorem 1 the left-hand side is zero, we have

$$\int_{S} \hat{\mathbf{t}}\cdot\mathbf{u}\,\mathrm{d}S = \sum_{\text{disl}} \int_{A_{\text{slip}}} (\mathbf{n}\cdot\hat{\boldsymbol{\sigma}}\cdot\mathbf{b})\,\mathrm{d}A_{\text{slip}}, \tag{3.6}$$

so that (3.3) and (3.6) again establish the identity (2.12). Using (3.3) and (3.6), the strain energy representations (2.4) and (2.11) therefore become

$$U_V = \frac{1}{2}\int_{\infty} \tilde{\boldsymbol{\sigma}}:\tilde{\boldsymbol{\varepsilon}}\,\mathrm{d}V - \frac{1}{2}\sum_{\text{disl}} \int_{A_{\text{slip}}} (\mathbf{n}\cdot\hat{\boldsymbol{\sigma}}\cdot\mathbf{b})\,\mathrm{d}A_{\text{slip}}. \tag{3.7}$$

4. Variational expressions

In the next section, which deals with dislocation equilibrium conditions, we need to express the strain energy variation corresponding to changes in dislocation positions. In this section we first elaborate on the variation of the surface integrals appearing on the right-hand sides of the energy expressions (2.4) and (2.11).

4.1. *Evaluation of the variation* $\delta(\int_S \bar{\mathbf{t}}\cdot\tilde{\mathbf{u}}\,\mathrm{d}S)$

We first consider the surface integral in (2.4), whose variation is

$$\delta\left(\int_S \bar{\mathbf{t}}\cdot\tilde{\mathbf{u}}\,\mathrm{d}S\right) = \int_S \delta\bar{\mathbf{t}}\cdot\tilde{\mathbf{u}}\,\mathrm{d}S + \int_S \bar{\mathbf{t}}\cdot\delta\tilde{\mathbf{u}}\,\mathrm{d}S. \tag{4.1}$$

From Fig. 1c, we have

$$\int_{\infty} \boldsymbol{\sigma} : \delta\boldsymbol{\varepsilon}\, \mathrm{d}V = \int_{V} \boldsymbol{\sigma} : \delta\boldsymbol{\varepsilon}\, \mathrm{d}V + \int_{S} \bar{\mathbf{t}} \cdot \delta\mathbf{u}\, \mathrm{d}S, \tag{4.2}$$

$$\int_{\infty} \delta\boldsymbol{\sigma} : \boldsymbol{\varepsilon}\, \mathrm{d}V = \int_{V} \delta\boldsymbol{\sigma} : \boldsymbol{\varepsilon}\, \mathrm{d}V + \int_{S} \delta\bar{\mathbf{t}} \cdot \mathbf{u}\, \mathrm{d}S, \tag{4.3}$$

as by the Gauss theorem, for example,

$$\int_{(\infty - V)} \boldsymbol{\sigma} : \delta\boldsymbol{\varepsilon}\, \mathrm{d}V = \int_{S} \bar{\mathbf{t}} \cdot \delta\mathbf{u}\, \mathrm{d}S. \tag{4.4}$$

The left-hand sides, as well as the volume integrals on the right-hand sides of (4.2) and (4.3) are by reciprocity equal, and therefore

$$\int_{S} \bar{\mathbf{t}} \cdot \delta\mathbf{u}\, \mathrm{d}S = \int_{S} \delta\bar{\mathbf{t}} \cdot \mathbf{u}\, \mathrm{d}S. \tag{4.5}$$

But

$$\int_{S} \bar{\mathbf{t}} \cdot \delta\tilde{\mathbf{u}}\, \mathrm{d}S = \int_{\infty} \bar{\boldsymbol{\sigma}} : \delta\bar{\boldsymbol{\varepsilon}}\, \mathrm{d}V = \int_{\infty} \delta\bar{\boldsymbol{\sigma}} : \bar{\boldsymbol{\varepsilon}}\, \mathrm{d}V = \int_{S} \delta\bar{\mathbf{t}} \cdot \tilde{\mathbf{u}}\, \mathrm{d}S, \tag{4.6}$$

and from (4.5) we also have

$$\int_{S} \bar{\mathbf{t}} \cdot \delta\tilde{\mathbf{u}}\, \mathrm{d}S = \int_{S} \delta\bar{\mathbf{t}} \cdot \tilde{\mathbf{u}}\, \mathrm{d}S, \tag{4.7}$$

so that the variation (4.1) becomes

$$\delta\left(\int_{S} \bar{\mathbf{t}} \cdot \tilde{\mathbf{u}}\, \mathrm{d}S\right) = 2 \int_{S} \bar{\mathbf{t}} \cdot \delta\tilde{\mathbf{u}}\, \mathrm{d}S. \tag{4.8}$$

We can express this in terms of the dislocation slip variation, by again using the Gauss theorem

$$\int_{\infty} \bar{\boldsymbol{\sigma}} : \delta\tilde{\boldsymbol{\varepsilon}}\, \mathrm{d}V = \int_{S} \bar{\mathbf{t}} \cdot \delta\tilde{\mathbf{u}}\, \mathrm{d}S - \sum_{\mathrm{disl}} \int_{\delta A_{\mathrm{slip}}} (\mathbf{n} \cdot \hat{\boldsymbol{\sigma}} \cdot \mathbf{b})\, \mathrm{d}(\delta A_{\mathrm{slip}}), \tag{4.9}$$

which gives

$$\int_S \bar{\mathbf{t}} \cdot \delta \tilde{\mathbf{u}} \, \mathrm{d}S = \sum_{\text{disl}} \int_{\delta A_{\text{slip}}} (\mathbf{n} \cdot \hat{\boldsymbol{\sigma}} \cdot \mathbf{b}) \, \mathrm{d}(\delta A_{\text{slip}}), \tag{4.10}$$

since the left-hand side of (4.9) is by Theorem 1 equal to zero. Similarly

$$\int_S \delta \bar{\mathbf{t}} \cdot \tilde{\mathbf{u}} \, \mathrm{d}S = \sum_{\text{disl}} \int_{A_{\text{slip}}} (\mathbf{n} \cdot \delta \hat{\boldsymbol{\sigma}} \cdot \mathbf{b}) \, \mathrm{d}A_{\text{slip}}, \tag{4.11}$$

so that, in view of (4.7), we also have

$$\sum_{\text{disl}} \int_{\delta A_{\text{slip}}} (\mathbf{n} \cdot \hat{\boldsymbol{\sigma}} \cdot \mathbf{b}) \, \mathrm{d}(\delta A_{\text{slip}}) = \sum_{\text{disl}} \int_{A_{\text{slip}}} (\mathbf{n} \cdot \delta \hat{\boldsymbol{\sigma}} \cdot \mathbf{b}) \, \mathrm{d}A_{\text{slip}}. \tag{4.12}$$

Finally, since the element of the slip variation increment $\mathrm{d}(\delta A_{\text{slip}})$ can be expressed as $\delta s \, \mathrm{d}l$, where δs is the perpendicular advance in the slip plane of the infinitesimal dislocation segment of length $\mathrm{d}l$, substitution of (4.10) into (4.8) gives

$$\delta\left(\int_S \bar{\mathbf{t}} \cdot \tilde{\mathbf{u}} \, \mathrm{d}S\right) = 2 \sum_{\text{disl}} \int_l (\mathbf{n} \cdot \hat{\boldsymbol{\sigma}} \cdot \mathbf{b}) \, \delta s \, \mathrm{d}l. \tag{4.13}$$

4.2. *Evaluation of the variation* $\delta(\int_S \hat{\mathbf{t}} \cdot \mathbf{u} \, \mathrm{d}S)$

We now consider the variation of the surface integral appearing in (2.11). Although it is clear that, in view of identity (2.12), the variations must be the same as well, it is of interest to establish this independently, with recourse only to the auxiliary loading $\hat{\mathbf{t}}$. Therefore, we start with

$$\delta\left(\int_S \hat{\mathbf{t}} \cdot \mathbf{u} \, \mathrm{d}S\right) = \int_S \delta \hat{\mathbf{t}} \cdot \mathbf{u} \, \mathrm{d}S + \int_S \hat{\mathbf{t}} \cdot \delta \mathbf{u} \, \mathrm{d}S. \tag{4.14}$$

Then

$$\int_\infty \tilde{\boldsymbol{\sigma}} : \delta \tilde{\boldsymbol{\varepsilon}} \, \mathrm{d}V = \int_V \tilde{\boldsymbol{\sigma}} : \delta \tilde{\boldsymbol{\varepsilon}} \, \mathrm{d}V + \int_S \hat{\mathbf{t}} \cdot \delta \tilde{\mathbf{u}} \, \mathrm{d}S, \tag{4.15}$$

since by the Gauss theorem

$$\int_{(\infty - V)} \tilde{\boldsymbol{\sigma}} : \delta\tilde{\boldsymbol{\varepsilon}}\, \mathrm{d}V = \int_S \hat{\mathbf{t}} \cdot \delta\tilde{\mathbf{u}}\, \mathrm{d}S, \tag{4.16}$$

and similarly

$$\int_\infty \delta\tilde{\boldsymbol{\sigma}} : \tilde{\boldsymbol{\varepsilon}}\, \mathrm{d}V = \int_V \delta\tilde{\boldsymbol{\sigma}} : \tilde{\boldsymbol{\varepsilon}}\, \mathrm{d}V + \int_S \delta\hat{\mathbf{t}} \cdot \tilde{\mathbf{u}}\, \mathrm{d}S. \tag{4.17}$$

But, the corresponding volume integrals in (4.15) and (4.17) are equal because of the reciprocity and generalized Hooke's law ($\tilde{\boldsymbol{\sigma}} = \mathbf{L} : \tilde{\boldsymbol{\varepsilon}}$ and $\delta\tilde{\boldsymbol{\sigma}} = \mathbf{L} : \delta\tilde{\boldsymbol{\varepsilon}}$). Consequently,

$$\int_S \hat{\mathbf{t}} \cdot \delta\tilde{\mathbf{u}}\, \mathrm{d}S = \int_S \delta\hat{\mathbf{t}} \cdot \tilde{\mathbf{u}}\, \mathrm{d}S \quad \text{and} \quad \int_S \hat{\mathbf{t}} \cdot \delta\mathbf{u}\, \mathrm{d}S = \int_S \delta\hat{\mathbf{t}} \cdot \mathbf{u}\, \mathrm{d}S, \tag{4.18}$$

since

$$\int_S \hat{\mathbf{t}} \cdot \delta\hat{\mathbf{u}}\, \mathrm{d}S = \int_V \hat{\boldsymbol{\sigma}} : \delta\hat{\boldsymbol{\varepsilon}}\, \mathrm{d}V = \int_V \delta\hat{\boldsymbol{\sigma}} : \hat{\boldsymbol{\varepsilon}}\, \mathrm{d}V = \int_S \delta\hat{\mathbf{t}} \cdot \hat{\mathbf{u}}\, \mathrm{d}S. \tag{4.19}$$

On the other hand, from

$$0 = \int_V \hat{\boldsymbol{\sigma}} : \delta\boldsymbol{\varepsilon}\, \mathrm{d}V = \int_S \hat{\mathbf{t}} \cdot \delta\mathbf{u}\, \mathrm{d}S - \sum_{\text{disl}} \int_{\delta A_{\text{slip}}} (\mathbf{n} \cdot \hat{\boldsymbol{\sigma}} \cdot \mathbf{b})\, \mathrm{d}(\delta A_{\text{slip}}), \tag{4.20}$$

we have

$$\int_S \hat{\mathbf{t}} \cdot \delta\mathbf{u}\, \mathrm{d}S = \sum_{\text{disl}} \int_{\delta A_{\text{slip}}} (\mathbf{n} \cdot \hat{\boldsymbol{\sigma}} \cdot \mathbf{b})\, \mathrm{d}(\delta A_{\text{slip}}), \tag{4.21}$$

and, in view of $(4.18)_2$, (4.14) becomes

$$\delta\left(\int_S \hat{\mathbf{t}} \cdot \mathbf{u}\, \mathrm{d}S\right) = 2 \sum_{\text{disl}} \int_l (\mathbf{n} \cdot \hat{\boldsymbol{\sigma}} \cdot \mathbf{b})\, \delta s\, \mathrm{d}l, \tag{4.22}$$

which is in agreement with the already established variation (4.13).

5. Dislocation equilibrium conditions

On assuming that a given population of fixed type and shape dislocations has its equilibrium configuration within the finite body V, the dislocation distribution is such that it minimizes the strain energy U_V (if equilibrium is stable), or maximizes it (if it is unstable). Since in general there may not be a unique equilibrium configuration, these minima or maxima can be local or absolute. In any case, the condition for equilibrium is the stationary value of the strain energy, $\delta U_V = 0$, which from (2.4) and (4.13), or (2.11) and (4.22), gives

$$\delta \tilde{U}_\infty - \sum_{\text{disl}} \int_l (\mathbf{n}\cdot\hat{\boldsymbol{\sigma}}\cdot\mathbf{b})\,\delta s\,\mathrm{d}l = 0. \tag{5.1}$$

We can express the infinite medium dislocation energy $\tilde{U}_\infty$ as the sum of the self energy $\tilde{U}_\infty^{\text{self}}$, resulting from the (infinite medium) stress and strain fields of all dislocations individually, and interaction energy $\tilde{U}_\infty^{\text{int}}$, resulting from the interaction of the stress and strain fields of various dislocations, i.e.

$$\tilde{U}_\infty = \frac{1}{2}\int_\infty \tilde{\boldsymbol{\sigma}}:\tilde{\boldsymbol{\varepsilon}}\,\mathrm{d}V = \tilde{U}_\infty^{\text{self}} + \tilde{U}_\infty^{\text{int}}. \tag{5.2}$$

Indeed, let $\boldsymbol{\sigma}_i$ and $\boldsymbol{\varepsilon}_i$ be the stress and strain fields of dislocation i in an infinite medium ($i = 1, 2, \ldots, n$-number of dislocations); then

$$\tilde{U}_\infty^{\text{self}} = \sum_{i=1}^{n} \frac{1}{2}\int_\infty \boldsymbol{\sigma}_i:\boldsymbol{\varepsilon}_i\,\mathrm{d}V \quad \text{and} \quad \tilde{U}_\infty^{\text{int}} = \sum_{i=1}^{n} \frac{1}{2}\int_\infty \Big(\sum_{j\neq i} \boldsymbol{\sigma}_j\Big):\boldsymbol{\varepsilon}_i\,\mathrm{d}V. \tag{5.3}$$

Since we consider dislocations to be of fixed size and shape, they can move along their slip planes only as "rigid" entities, and if the medium is elastically isotropic, $\tilde{U}_\infty^{\text{self}}$ is constant regardless of dislocation positions, so that $\delta\tilde{U}_\infty^{\text{self}} = 0$. (Note also that divergence of $\tilde{U}_\infty$ which comes from the dislocation core energy is present only in the $\tilde{U}_\infty^{\text{self}}$ part of the energy; and since $\delta\tilde{U}_\infty^{\text{self}} = 0$, the variational expressions here developed do not depend on the scheme by which the core energy is represented). Variation of the interaction energy $\delta\tilde{U}_\infty^{\text{int}}$ can be expressed as

$$\delta\tilde{U}_\infty^{\text{int}} = \sum_{i=1}^{n} \int_\infty \Big(\sum_{j\neq i} \boldsymbol{\sigma}_j\Big):\delta\boldsymbol{\varepsilon}_i\,\mathrm{d}V, \tag{5.4}$$

which, by using Gauss's formula can be rewritten in short as

$$\delta\tilde{U}_\infty^{\text{int}} = -\sum_{\text{disl}} \int_l (\mathbf{n}\cdot\tilde{\boldsymbol{\sigma}}^{\text{int}}\cdot\mathbf{b})\,\delta s\,\mathrm{d}l. \tag{5.5}$$

Here $\tilde{\boldsymbol{\sigma}}^{\text{int}} = \Sigma_{j\neq i}\boldsymbol{\sigma}_j$ is the stress along dislocation i, caused by all other dislocations j (interaction stress), while as before $\delta s\,\mathrm{d}l$ is the infinitesimal element of the slip increment δA_{slip} along a dislocation of length l, and δs the corresponding perpendicular advance of a dislocation point. This, of course, can also be deduced from the Peach-Koehler representation [6, 7] of the dislocation interaction force and associated expression for the interaction energy. Introducing (5.5) into (5.1) therefore yields

$$\sum_{\text{disl}} \int_l [\mathbf{n} \cdot (\tilde{\boldsymbol{\sigma}}^{\text{int}} + \hat{\boldsymbol{\sigma}}) \cdot \mathbf{b}] \, \delta s \, \mathrm{d}l = \sum_{\text{disl}} \int_l \mathrm{d}f_{\text{gl}} \, \delta s = 0, \tag{5.6}$$

in which $\mathrm{d}f_{\text{gl}} = [\mathbf{n} \cdot (\tilde{\boldsymbol{\sigma}}^{\text{int}} + \hat{\boldsymbol{\sigma}}) \cdot \mathbf{b}] \, \mathrm{d}l$ is the magnitude of the glide force on a dislocation element $\mathrm{d}l$ (which is normal to dislocation line), resulting from the interaction of dislocation with all others, as represented by interaction stress $\tilde{\boldsymbol{\sigma}}^{\text{int}}$, and from the auxiliary stress field $\hat{\boldsymbol{\sigma}}$.

We note that at each infinitesimal segment $\mathrm{d}l$ of the dislocation line, there is also a contribution to the glide force resulting from the interaction of that segment with other segments of the same dislocation (a self-glide force). Since we here consider variations in dislocation positions which preserve dislocation size and shape, the self-glide forces are constant during the variation, and therefore do not participate in the stationary condition (5.6). This is also clear since we have already taken $\delta \tilde{U}_{\infty}^{\text{self}} = 0$, and it is the change in $\tilde{U}_{\infty}^{\text{self}}$ that is associated with the self-glide force. For more details on this issue, we refer to [2].

On returning to (5.6), since variations of dislocation positions among dislocations are independent, (5.6) gives the equilibrium condition for each dislocation individually,

$$\int_l \mathrm{d}f_{\text{gl}} \, \delta s = 0. \tag{5.7}$$

For example, if the variation of a dislocation position is defined by its ("rigid body") translation $\delta \mathbf{r} = \delta r \, \mathbf{r}_0$, where δr is the magnitude of translation and $\mathbf{r}_0$ its direction, then $\mathrm{d}f_{\text{gl}} \, \delta s = \mathbf{df}_{\text{gl}} \cdot \delta r \, \mathbf{r}_0$; and since δr is constant along the dislocation line, (5.7) gives

$$\int_l \mathbf{df}_{\text{gl}} \cdot \mathbf{r}_0 = 0, \tag{5.8}$$

which means that the sum of the glide force projections in the translation direction $\mathbf{r}_0$ is equal to zero. Since $\mathbf{r}_0$ can be any direction in the slip plane, (5.8) in fact gives

$$\int_l \mathbf{df}_{\text{gl}} = 0, \tag{5.9}$$

i.e. the vector sum of all glide forces is zero for each dislocation. Similarly, by assuming that the dislocation in its slip plane instantaneously rotates about an arbitrary point P, $\delta\mathbf{r} = \delta\varphi\mathbf{n}\times\mathbf{x}$, $\delta\varphi$ being the virtual rotation and $\mathbf{x}$ the position vector of the dislocation point relative to P, we have $\mathrm{d}f_{\mathrm{gl}}\delta s = \mathrm{d}\mathbf{f}_{\mathrm{gl}}\cdot(\mathbf{n}\times\mathbf{x})\delta\varphi = \mathbf{n}\cdot(\mathbf{x}\times\mathrm{d}\mathbf{f}_{\mathrm{gl}})\delta\varphi$, and (5.7) gives

$$\int_l \mathbf{x}\times\mathrm{d}\mathbf{f}_{\mathrm{gl}} = \mathbf{0}, \tag{5.10}$$

which means that the resulting moment of the glide forces is zero for every dislocation. Together, (5.9) and (5.10), therefore indicate that the glide forces of each dislocation represent a balanced set of self-equilibrated forces.

Appendix

A slight modification in some of the derivation is needed when we consider the plane strain situation and edge dislocations which do not form the loops within the body V (pairs of opposite-sign dislocations on the same slip plane). In that case there is a jump of displacement $\tilde{\mathbf{u}}$ not only within V, but also within $(\infty - V)$, because A_{slip} extends along the slip plane from each dislocation to infinity (Fig. 4). Therefore, in applying the Gauss theorem to the $(\infty - V)$ body,

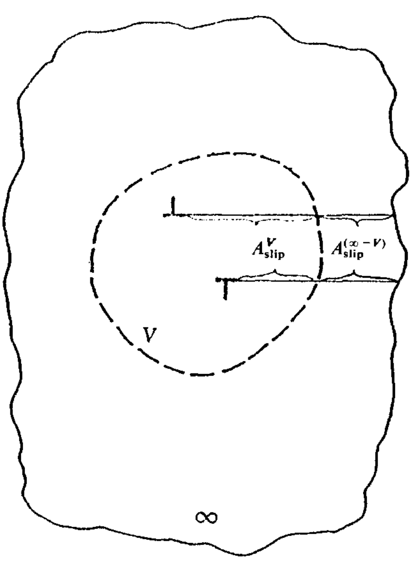


Fig. 4. Edge dislocations in plane strain: slip surface consists of the portion within the body V, A^V_{slip}, and the remaining part which extends to infinity, $A^{(\infty-V)}_{\mathrm{slip}}$; when dislocations move within V, only A^V_{slip} changes, so that $\delta A^{(\infty-V)}_{\mathrm{slip}} = 0$.

we have, for example,

$$\int_{(\infty - V)} \boldsymbol{\sigma} : \boldsymbol{\varepsilon} \, \mathrm{d}V = \int_S \bar{\mathbf{t}} \cdot \mathbf{u} \, \mathrm{d}S - \sum_{\mathrm{disl}} \int_{A_{\mathrm{slip}}^{(\infty - V)}} (\mathbf{n} \cdot \boldsymbol{\sigma} \cdot \mathbf{b}) \, \mathrm{d}A_{\mathrm{slip}}^{(\infty - V)}, \tag{A.1}$$

and therefore, in place of (4.2), the strain energy within V is given by

$$U_V = \frac{1}{2} \int_{\infty} \tilde{\boldsymbol{\sigma}} : \tilde{\boldsymbol{\varepsilon}} \, \mathrm{d}V - \frac{1}{2} \int_S \bar{\mathbf{t}} \cdot \tilde{\mathbf{u}} \, \mathrm{d}S + \frac{1}{2} \sum_{\mathrm{disl}} \int_{A_{\mathrm{slip}}^{(\infty - V)}} (\mathbf{n} \cdot \boldsymbol{\sigma} \cdot \mathbf{b}) \, \mathrm{d}A_{\mathrm{slip}}^{(\infty - V)}. \tag{A.2}$$

Similar modifications are needed in the variational analysis. Since $\delta A_{\mathrm{slip}}^{(\infty - V)} \equiv 0$, because during the variation of their positions dislocations remain within V, (4.2) holds unchanged, while (4.3) is replaced by

$$\int_{\infty} \delta\boldsymbol{\sigma} : \boldsymbol{\varepsilon} \, \mathrm{d}V = \int_V \delta\boldsymbol{\sigma} : \boldsymbol{\varepsilon} \, \mathrm{d}V + \int_S \delta\bar{\mathbf{t}} \cdot \mathbf{u} \, \mathrm{d}S - \sum_{\mathrm{disl}} \int_{A_{\mathrm{slip}}^{(\infty - V)}} (\mathbf{n} \cdot \delta\boldsymbol{\sigma} \cdot \mathbf{b}) \, \mathrm{d}A_{\mathrm{slip}}^{(\infty - V)}. \tag{A.3}$$

Consequently, the variation of (A.2) becomes

$$\delta U_V = \delta\left(\frac{1}{2} \int_{\infty} \tilde{\boldsymbol{\sigma}} : \tilde{\boldsymbol{\varepsilon}} \, \mathrm{d}V\right) - \int_S \bar{\mathbf{t}} \cdot \delta\tilde{\mathbf{u}} \, \mathrm{d}S, \tag{A.4}$$

which is exactly as previously shown. The rest of the analysis remains as presented in the paper. Of course, if all dislocations are pairs of opposite signs forming the loop structures, no modification is needed at all, since $A_{\mathrm{slip}}^{(\infty - V)} = 0$. Similar remarks apply to the formulation which uses the auxiliary problem with traction $\hat{\mathbf{t}}$ on S.

Therefore, (A.4) leads to (5.6) and (5.7), and since δs is independent among all individual dislocations, we have $f_{\mathrm{gl}} = 0$ for each dislocation. By denoting the shear stress over the slip plane of dislocation in the direction of its Burgers vector by τ, the resulting glide force on a dislocation can be expressed as $l(\tilde{\tau}^{\mathrm{int}} + \hat{\tau})b$, where l is the (infinite) length of dislocation, and therefore for equilibrium

$$\tilde{\tau}^{\mathrm{int}} + \hat{\tau} = 0, \tag{A.5}$$

i.e. the shear stress in the slip plane of a dislocation, resulting from its interaction with other dislocations and auxiliary applied traction, is zero for every dislocation. For application of this result and determination of some characteristic equilibrium distributions of large number of dislocations, we refer to [5].

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