Macroscopic stress and strain in a doubly periodic array of dislocation dipoles*

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Abstract

It is known that in two-dimensional periodic arrays of dislocations the summation of the periodic image fields is conditionally convergent. This is due to the long range character of the elastic fields of dislocations. As a result, the stress field obtained for a doubly periodic array of dislocation dipoles may contain a spurious constant stress that depends on the adopted summation scheme. In the present work, we provide, based on micromechanical considerations, a simple physical explanation of the origin of the conditional convergence of lattice sums of image interactions. In this context, the spurious stresses are found in a closed form for an arbitrary elastic anisotropy, and this is achieved without using the stress field of an individual dislocation. An alternative procedure is also developed where the macroscopic spurious stresses are determined using the solution of the Eshelby's inclusion problem.

Keywords: dislocation dynamics; conditional convergence; micromechanics; Eshelby's inclusion problem

1 Introduction

Dislocation dynamics (DD) simulation methods have been extensively employed over the last decades to study the dynamic behavior of dislocations on a mesoscopic scale and to investigate the fundamental aspects of plastic deformation, with a view towards connecting the physics of dislocations with the evolution of strength and strain hardening in crystalline materials. Three-dimensional (3D) DD models have been mostly used to examine strain

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hardening due to dislocation forest interactions [1–3] and individual dislocation-defect interactions [4–7]. However, for complex problems, the use of 2D DD models is common due to the high computational cost of 3D DD [8]. Although 2D DD simulations provide just a simplification of the 3D dislocation microstructures in real crystals, they have been extensively applied to account for many aspects of dislocation physics. Indeed, 2D models have been successfully employed to provide insight into a variety of problems including discrete dislocation plasticity [9], dislocation-crack interaction [10, 11], modeling of persistent slip bands [12], plasticity in thin films [13, 14], fatigue crack growth in single crystals [15], and size effects in fracture [16]. While the 2D DD simulations typically focus on edge dislocations, screw dislocations have also been considered, for instance, in [17].

In many cases, periodic boundary conditions in one or both directions are used for microscale DD simulations and in particular for studying the dislocation interaction in bulk crystals [18]. As noted by Cai et al. [18], the principal advantage of periodic boundary conditions for modelling crystal defects is that they eliminate surfaces and preserve translational invariance, the fundamental property of the crystal lattice. Under these circumstances, for each defect in the unit cell, one must also account for the fields due to its replicas in all other cells in the array. In practice, in 2D DD, the enforcement of periodic boundary conditions can be readily achieved by performing an analytical summation over infinitely long rows or columns of dislocations in one direction, followed by a numerical summation of the contributions of each wall in the other direction [19, 20]. However, even though the self-stress fields decay rapidly with the distance from the dislocation, walls of dislocations have been observed to give rise to very long-range effects [19].

An important consequence related to the intrinsic long-range character of dislocation interaction is the *conditional convergence* of the lattice sums of the image fields. In fact, as it has been shown by Cai et al. [18], see also Kuykendall and Cai [20], the result of the lattice sum depends on the pertinent summation scheme. For instance, the stress field obtained by the summation along the x_1-direction followed by the summation in the x_2-direction is in general different than that obtained by the summation along the x_2- and then along the x_1-direction. In particular, the resulting stress field may contain a spurious constant stress for a zero total Burgers vector in the simulation cell and a spurious linear stress field for a non-zero total Burgers vector, cf. [20]. As a remedy, Cai et al. [18] have developed a method in which the spurious stresses are computed numerically by introducing ghost dislocations at the cell boundaries. Recently, Kuykendall and Cai [20] have proposed an alternative mathematical procedure for the 2D case, where the spurious stresses are found analytically by integrating twice the sum of the second derivatives of the stress field and noting that the latter is absolutely convergent under periodic boundary conditions. Importantly, these spurious stresses discussed above contribute to the Peach–Koehler forces and hence may affect the DD simulation results.

In the present work, we develop, based on simple micromechanical considerations, an alternative approach for the prediction of the spurious stresses in a doubly periodic array of dislocation dipoles. Consequently, we only consider the case of a zero total Burgers vector in a simulation cell. Configurations with a non-zero total Burgers vector are not considered here since they are not compatible with the doubly periodic boundary conditions so that the micromechanical framework adopted in this work is not applicable. Although the basic idea of our approach is rather simple, a rigorous derivation of the final results requires introduction of several intermediate concepts and relationships. Accordingly, the basic idea is briefly outlined below as a guide for the technical developments presented in subsequent sections.

We adopt a micromechanical point of view so that the general structure of the solution for a doubly periodic array of dislocation dipoles can be deduced without performing the summation and even without specifying the solution for a single dislocation. Specifically, the local stress $\boldsymbol{\sigma}(\boldsymbol{x})$ in the periodic unit cell can be decomposed into a (constant) macroscopic stress $\boldsymbol{\Sigma}$ and a periodic fluctuation $\tilde{\boldsymbol{\sigma}}(\boldsymbol{x})$,

$$\boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{\Sigma} + \tilde{\boldsymbol{\sigma}}(\boldsymbol{x}), \tag{1}$$

where the volume average of the fluctuation $\tilde{\boldsymbol{\sigma}}(\boldsymbol{x})$ is equal to zero. Further, assuming that the elastic moduli tensor $\mathbb{L}$ is homogeneous within the cell, the macroscopic stress $\boldsymbol{\Sigma}$ satisfies the macroscopic constitutive equation,

$$\boldsymbol{\Sigma} = \mathbb{L}[\boldsymbol{E}^{\mathrm{e}}] = \mathbb{L}[\boldsymbol{E} - \boldsymbol{E}^{\mathrm{p}}], \tag{2}$$

where $\boldsymbol{E}$ is the macroscopic strain with $\boldsymbol{E}^{\mathrm{e}}$ and $\boldsymbol{E}^{\mathrm{p}}$ being its elastic and plastic parts, respectively, the latter straightforwardly determined in terms of the Burgers vectors and geometrical arrangement of the dislocation dipoles.

The fluctuation stress $\tilde{\boldsymbol{\sigma}}(\boldsymbol{x})$ can now be interpreted as the stress corresponding to a zero macroscopic stress $\boldsymbol{\Sigma}$ and thus caused solely by the dislocations in the primary cell and in its periodic replicas. In fact, for DD simulations, it is the fluctuation stress $\tilde{\boldsymbol{\sigma}}(\boldsymbol{x})$ that is of actual interest, since the constant macroscopic stress $\boldsymbol{\Sigma}$ would typically be prescribed, either directly or indirectly through (2). However, as discussed above, a direct summation of stress fields of individual dislocation dipoles is conditionally convergent [20] and may introduce a constant spurious stress. That spurious stress can be now interpreted as the *macroscopic* stress $\boldsymbol{\Sigma}$, and its origin is briefly illustrated below, while a detailed analysis is the objective of the present work and is pursued in the subsequent sections.

Consider thus a one-dimensional periodic array of dislocation dipoles. As illustrated in Fig. 1, the dipoles may introduce an inelastic in-plane (interior) strain component so that in-plane stresses must be applied to ensure the overall compatibility, as indicated by the arrows in Fig. 1. Note that the configuration shown in the right-most figure corresponds to the stress field obtained by an infinite summation of the contributions of individual dislocation dipoles along the horizontal direction. The stress field for a doubly periodic array of dipoles would then be obtained by a second summation in the vertical direction, and the in-plane stresses mentioned above would contribute to the final macroscopic stress. Of course, a different macroscopic stress would be obtained if the order of summations was reversed which is mathematically interpreted as the conditional convergence of the summation scheme. Note that, in the configuration shown in Fig. 1, the local stresses are equal to zero far from the array of dipoles. The macroscopic stresses corresponding to the two summation schemes are thus different because different conditions are imposed on the stress fields in the two cases.

Furthermore, it is also illustrated in Fig. 1 that the out-of-plane (exterior) inelastic strain components, for instance, the shear strain, do not introduce any macroscopic stresses,

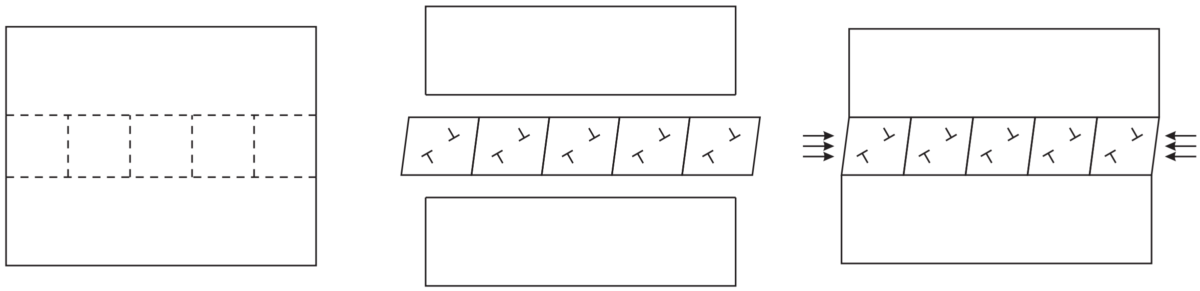

Figure 1: Origin of macroscopic stresses in a periodic array of dislocation dipoles.

as they are fully accommodated by a relative displacement of the upper half-space with respect to the lower half-space. In fact, some configurations of dislocation dipoles do not produce any spurious macroscopic stresses, and this was probably the reason that the problem of conditional convergence and the related spurious stresses had been initially overlooked by the dislocation dynamics community, as noted by Cai et al. [18].

The original contribution of this work and its main results are the following:

(i) We provide a physical explanation of the origin of the conditional convergence by showing that each summation scheme corresponds to specific conditions for the stresses at infinity. As a result, the stress fields obtained by direct summation of the contributions of individual dislocation dipoles are not pure fluctuations, but also contain a macroscopic stress which depends on the conditions imposed on the far-field stresses by the summation scheme.

(ii) We show that the spurious macroscopic stress can be determined without knowing the stress field of an individual dislocation. This is in contrast to the solution provided by Kuykendall and Cai [20] who determine the spurious stress by taking adequate limits of the fields generated by individual dislocations.

(iii) As a consequence of (ii), the spurious macroscopic stress corresponding to the summation scheme involving infinite summation in one direction followed by summation in the other direction is found in a closed form for an arbitrary elastic anisotropy.

(iv) We also consider yet another summation scheme in which summation is truncated in all directions at a fixed distance from the primary cell. The corresponding spurious macroscopic stress is then determined from the Eshelby's solution of an elliptical inclusion in an elastic matrix. We also show that the results mentioned in (iii) are recovered as the limit cases of the Eshelby solution when summation is performed within an elliptical region of aspect ratio tending to zero or infinity.

The paper is organized as follows. In Section 2, the average stress and strain are defined for a volume containing dislocation dipoles, and elastic and plastic parts of the average strain are identified. A one-dimensional periodic array of dislocation dipoles is considered in Section 3, and the average stress and strain are determined for a volume containing the dipole and for a defect-free volume. In Section 4, closed-form formulae are derived for the macroscopic stress and strain in a doubly periodic array of dislocation dipoles. Finally, in Section 5, an alternative summation scheme is introduced, for which the macroscopic stress can be obtained using the solution of the Eshelby's inclusion problem.

2 Average stress and strain

In this section, we consider a volume V of arbitrary shape in the (x_1, x_2)-plane that contains an arbitrary ensemble of N dislocation dipoles with straight dislocation lines parallel to the x_3-axis and slip planes defined by unit normal vectors $\boldsymbol{\nu}^{(i)}$ within the (x_1, x_2)-plane (Fig. 2). Each i-th dipole is formed by a dislocation with the Burgers vector $\boldsymbol{b}^k = \boldsymbol{b}^{(i)}$ and an opposite dislocation with the Burgers vector $\boldsymbol{b}^{k+1} = -\boldsymbol{b}^{(i)}$ at distance $d^{(i)}$. Consequently, the total net Burgers vector is zero in the volume V,

$$\sum_{k=1}^{2N} \boldsymbol{b}^k = 0. \tag{3}$$

It is noted that no restrictions are imposed on the orientation of the Burgers vectors $\boldsymbol{b}^{(i)}$, i.e., they can be arbitrary vectors in 3D, so that the dislocations can be of the edge, screw or mixed type. In the present circumstances, the volume is essentially under a combined state of plane and antiplane strain conditions where all the local variables depend upon a 2D position vector $\boldsymbol{x} = x_1\boldsymbol{e}_1 + x_2\boldsymbol{e}_2$.

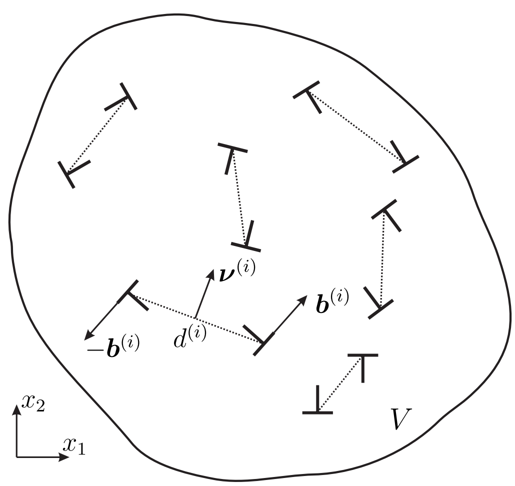

Figure 2: Ensemble of dislocation dipoles inside the volume V.

It can be easily verified that an arbitrary arrangement of dislocations with the total net Burgers vector equal to zero, as in Eq. (3), can be replaced by an equivalent arrangement of dislocation dipoles of opposite Burgers vectors. Accordingly, the present analysis is applicable in that more general case as well.

The local stress, strain and displacement fields in the volume V can be found by superposition of the corresponding fields imposed by the boundary conditions on ∂V, denoted by a superimposed hat, and the fields by the individual dislocations, cf. [19],

$$\boldsymbol{\sigma}(\boldsymbol{x}) = \hat{\boldsymbol{\sigma}}(\boldsymbol{x}) + \sum_{k=1}^{2N} \boldsymbol{\sigma}^k(\boldsymbol{x}), \quad \boldsymbol{\varepsilon}(\boldsymbol{x}) = \hat{\boldsymbol{\varepsilon}}(\boldsymbol{x}) + \sum_{k=1}^{2N} \boldsymbol{\varepsilon}^k(\boldsymbol{x}), \quad \boldsymbol{u}(\boldsymbol{x}) = \hat{\boldsymbol{u}}(\boldsymbol{x}) + \sum_{k=1}^{2N} \boldsymbol{u}^k(\boldsymbol{x}). \quad (4)$$

The average stress $\bar{\boldsymbol{\sigma}}$ and the average strain $\bar{\boldsymbol{\varepsilon}}$ in the volume V are defined in terms of the boundary data as [21]

$$\bar{\boldsymbol{\sigma}} = \frac{1}{V} \int_{\partial V} \frac{1}{2} (\boldsymbol{t} \otimes \boldsymbol{x} + \boldsymbol{x} \otimes \boldsymbol{t}) \, \mathrm{d}S, \qquad \bar{\boldsymbol{\varepsilon}} = \frac{1}{V} \int_{\partial V} \frac{1}{2} (\boldsymbol{u} \otimes \boldsymbol{n} + \boldsymbol{n} \otimes \boldsymbol{u}) \, \mathrm{d}S, \quad (5)$$

where $\boldsymbol{n}$ is the outward unit normal, and $\boldsymbol{t} = \boldsymbol{\sigma}\boldsymbol{n}$ is the traction acting on ∂V. For simplicity, the symbol V is used to denote both the domain and its measure, in the latter case regarded as a volume per unit length in the x_3-direction. Note that the dependence of all quantities upon the variable $\boldsymbol{x}$ will be explicitly indicated only when needed.

Employing the divergence theorem, the boundary integrals in (5) can be transformed to the corresponding volume integrals under the assumption of mechanical equilibrium in V and by observing that the displacement field is continuous in V except at the slip planes $S^{(i)}$ of the individual dislocation dipoles. The average stress and strain are then equivalently given by [21]

$$\bar{\boldsymbol{\sigma}} = \frac{1}{V} \int_V \boldsymbol{\sigma} \, \mathrm{d}V, \qquad \bar{\boldsymbol{\varepsilon}} = \frac{1}{V} \left(\int_{V \setminus S} \boldsymbol{\varepsilon} \, \mathrm{d}V + \int_S \frac{1}{2} (\llbracket \boldsymbol{u} \rrbracket \otimes \boldsymbol{n} + \boldsymbol{n} \otimes \llbracket \boldsymbol{u} \rrbracket) \, \mathrm{d}S \right), \quad (6)$$

where $\llbracket \boldsymbol{u} \rrbracket$ denotes the displacement jump across the discontinuity surface S with $\boldsymbol{n}$ being the local normal to S, and S is here the union of the individual slip planes $S^{(i)}$. Note that the volume integrals in (6) is to be considered in the Cauchy Principal Value (CPV) sense due to the Cauchy type singularities induced by the individual dislocations.

For a fixed configuration of dislocations, the (incremental) material response is elastic in the whole volume V, so that the local stress and strain are related by $\boldsymbol{\sigma} = \mathbb{L}[\boldsymbol{\varepsilon}]$, where $\mathbb{L}$ is the fourth-order elasticity tensor which is assumed positive definite and thus invertible. Assuming further that $\mathbb{L}$ is *homogeneous* in V, the volume integral of strain $\boldsymbol{\varepsilon}$ in $(6)_2$ is identified as the average elastic strain $\bar{\boldsymbol{\varepsilon}}^{\mathrm{e}}$ that is related to the average stress $\bar{\boldsymbol{\sigma}}$ by the constitutive relationship $\bar{\boldsymbol{\sigma}} = \mathbb{L}[\bar{\boldsymbol{\varepsilon}}^{\mathrm{e}}]$,

$$\frac{1}{V} \int_{V \setminus S} \boldsymbol{\varepsilon} \, \mathrm{d}V = \frac{1}{V} \int_{V \setminus S} \mathbb{L}^{-1}[\boldsymbol{\sigma}] \, \mathrm{d}V = \mathbb{L}^{-1} \left[\frac{1}{V} \int_V \boldsymbol{\sigma} \, \mathrm{d}V \right] = \mathbb{L}^{-1} [\bar{\boldsymbol{\sigma}}] = \bar{\boldsymbol{\varepsilon}}^{\mathrm{e}}, \quad (7)$$

where the volume integral of $\boldsymbol{\sigma}$ is considered in CPV sense. The second term in $(6)_2$ is thus identified as the average eigenstrain $\bar{\boldsymbol{\varepsilon}}^{\mathrm{p}} = \bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}}^{\mathrm{e}}$,

$$\bar{\boldsymbol{\varepsilon}}^{\mathrm{p}} = \frac{1}{V} \sum_{i=1}^{N} \int_{S^{(i)}} \frac{1}{2} \big(\llbracket \boldsymbol{u} \rrbracket \otimes \boldsymbol{n} + \boldsymbol{n} \otimes \llbracket \boldsymbol{u} \rrbracket \big) \mathrm{d}S = \frac{1}{2V} \sum_{i=1}^{N} d^{(i)} \left(\boldsymbol{b}^{(i)} \otimes \boldsymbol{\nu}^{(i)} + \boldsymbol{\nu}^{(i)} \otimes \boldsymbol{b}^{(i)} \right), \quad (8)$$

where the integral over S in $(6)_2$ has been split to the sum of integrals over the slip planes $S^{(i)}$ of individual dipoles, and has been further transformed by noting that $\boldsymbol{n} = \boldsymbol{\nu}^{(i)}$ and

$[\![\boldsymbol{u}]\!] = \boldsymbol{b}^{(i)}$, both being constant along $S^{(i)}$. Now, considering that the dislocation dipoles were created by Frank–Read sources, the average eigenstrain $\bar{\boldsymbol{\varepsilon}}^{\mathrm{p}}$ can be interpreted as the plastic strain, induced by motion of dislocations, measured with respect to the dislocation-free configuration [19].

Concluding, the average strain $\bar{\boldsymbol{\varepsilon}}$ has been decomposed into its elastic and plastic parts, $\bar{\boldsymbol{\varepsilon}} = \bar{\boldsymbol{\varepsilon}}^{\mathrm{e}} + \bar{\boldsymbol{\varepsilon}}^{\mathrm{p}}$, and the average stress and strain are related by the usual elastic constitutive relationship,

$$\bar{\boldsymbol{\sigma}} = \mathbb{L}\left[\bar{\boldsymbol{\varepsilon}}^{\mathrm{e}}\right] = \mathbb{L}\left[\bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}}^{\mathrm{p}}\right]. \tag{9}$$

3 Single array of dislocation dipoles

3.1 Preliminaries

Consider now a one-dimensional periodic array of dislocation dipoles with spacing L (Fig. 3). This configuration will be called a *string of dislocation dipoles* to distinguish it from the doubly periodic array of dipoles to be discussed later. Each dipole is formed by two infinitely long dislocation lines, with Burgers vector $\pm\boldsymbol{b}$, parallel to the out-of-plane vector $\boldsymbol{r}$ and separated by a distance d. It is remarked that the Burgers vector $\boldsymbol{b}$ may have nonzero in-plane and out-of-plane components, i.e., in general it has a 3D character. The array of dipoles is characterized by a unit vector $\boldsymbol{\nu}$ normal to the slip-plane with $\boldsymbol{\nu} \cdot \boldsymbol{r} = 0$, and a unit vector $\boldsymbol{p}$ defining the direction of periodicity. In addition, we define the vector $\boldsymbol{m}$ normal to the array of dipoles from the relation: $\boldsymbol{r} = \boldsymbol{p} \times \boldsymbol{m}$.

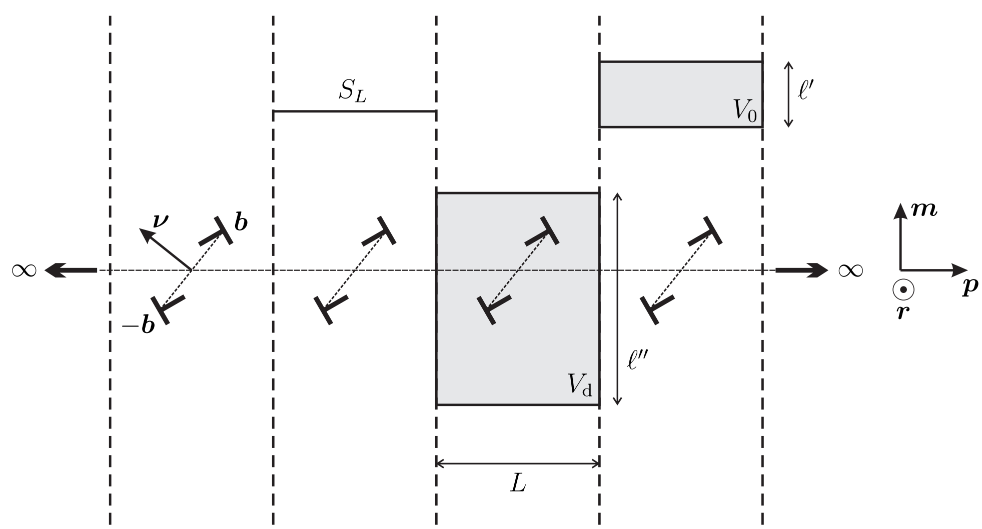

Figure 3: Periodic array (string) of dislocation dipoles. Two types of volumes are considered, both spanning exactly one period along the direction of periodicity: (i) V_0 which is free of defects and (ii) V_d which contains the dislocation dipole.

The stress field produced by the string of dislocation dipoles can be obtained by an infinite summation of the contributions of all dislocations in the $\boldsymbol{p}$-direction,

$$\boldsymbol{\sigma}(\boldsymbol{x}) = \sum_{i=-\infty}^{+\infty} \left[\boldsymbol{\sigma_b}(\boldsymbol{x} - \boldsymbol{x}^+ - iL\boldsymbol{p}) - \boldsymbol{\sigma_b}(\boldsymbol{x} - \boldsymbol{x}^- - iL\boldsymbol{p}) \right], \tag{10}$$

where $\boldsymbol{\sigma_b}(\boldsymbol{x})$ is the stress field of a single dislocation located at $\boldsymbol{x} = \boldsymbol{0}$ with Burgers vector $\boldsymbol{b}$, and $\boldsymbol{x}^+$ and $\boldsymbol{x}^-$ are the positions of the dislocations forming the dipole in the primary cell. It is noted that this summation can be performed analytically in closed form (see e.g. [19,20]). However, it is stressed that in our analysis the knowledge of such local stress field is not needed.

Note that in (10) we include only the stresses due to the dislocations forming the string, thus no external stresses are considered. However, for a volume V_{d} containing a single dipole (Fig. 3), the stress field can be equivalently considered to be a superposition of the stress due to the dislocations contained in V_{d} and the stress imposed by the boundary conditions on ∂V_{d}, the latter resulting from the dislocations outside V_{d} and corresponding to $\hat{\boldsymbol{\sigma}}$ in (4).

Since the stress field of a straight dislocation behaves as r^{-1} at large r (r being the distance from the dislocation), whereas the stress field of a dislocation dipole behaves as r^{-2} [19], we conclude that the pertinent infinite array of dislocation dipoles will not produce long range stresses in the $\boldsymbol{m}$-direction. Thus, we can write

$$\boldsymbol{\sigma}(\boldsymbol{x}) \to \boldsymbol{0} \quad \text{as} \quad \boldsymbol{x} \cdot \boldsymbol{m} \to \pm\infty. \tag{11}$$

Moreover, due to periodicity the following relations hold for the displacements and tractions:

$$\boldsymbol{u}(\boldsymbol{x}) = \boldsymbol{u}(\boldsymbol{x} + L\boldsymbol{p}), \quad \boldsymbol{t}^{(-\boldsymbol{p})}(\boldsymbol{x}) = -\boldsymbol{t}^{(\boldsymbol{p})}(\boldsymbol{x} + L\boldsymbol{p}), \tag{12}$$

where $\boldsymbol{t}^{(\boldsymbol{n})} = \boldsymbol{\sigma n}$ denotes the traction associated with normal $\boldsymbol{n}$.

3.2 Interior-exterior decomposition of the average stress and strain

The stress and strain tensors, and in particular the average stress and strain defined in (6), can be uniquely decomposed into their interior (P) and exterior (A) parts relative to a surface parallel to the string of dipoles represented by the normal vector $\boldsymbol{m}$, so that [22,23]

$$\bar{\boldsymbol{\sigma}} = \bar{\boldsymbol{\sigma}}_{\mathrm{P}} + \bar{\boldsymbol{\sigma}}_{\mathrm{A}}, \quad \bar{\boldsymbol{\varepsilon}} = \bar{\boldsymbol{\varepsilon}}_{\mathrm{P}} + \bar{\boldsymbol{\varepsilon}}_{\mathrm{A}}, \tag{13}$$

where the respective interior and exterior parts are defined as

$$\bar{\boldsymbol{\sigma}}_{\mathrm{P}} = \mathbb{P}_{\mathrm{P}}[\bar{\boldsymbol{\sigma}}], \quad \bar{\boldsymbol{\sigma}}_{\mathrm{A}} = \mathbb{P}_{\mathrm{A}}[\bar{\boldsymbol{\sigma}}], \tag{14}$$

$$\bar{\boldsymbol{\varepsilon}}_{\mathrm{P}} = \mathbb{P}_{\mathrm{P}}[\bar{\boldsymbol{\varepsilon}}], \quad \bar{\boldsymbol{\varepsilon}}_{\mathrm{A}} = \mathbb{P}_{\mathrm{A}}[\bar{\boldsymbol{\varepsilon}}], \tag{15}$$

with $\mathbb{P}_{\mathrm{P}}$ and $\mathbb{P}_{\mathrm{A}}$ being fourth-order projection tensors given as [22]

$$\mathbb{P}_{\mathrm{A}} = \boldsymbol{I} \boxdot (\boldsymbol{m} \otimes \boldsymbol{m}) + (\boldsymbol{m} \otimes \boldsymbol{m}) \boxdot \boldsymbol{I} - \boldsymbol{m} \otimes \boldsymbol{m} \otimes \boldsymbol{m} \otimes \boldsymbol{m}, \tag{16}$$

$$\mathbb{P}_{\rm P} = \boldsymbol{I} \boxdot \boldsymbol{I} - \mathbb{P}_{\rm A}. \tag{17}$$

Here, the tensorial product $\boxdot$ is defined as $\boldsymbol{A} \boxdot \boldsymbol{B}[\boldsymbol{C}] = \frac{1}{2}\left(\boldsymbol{A}\boldsymbol{C}\boldsymbol{B}^T + \boldsymbol{A}\boldsymbol{C}^T\boldsymbol{B}^T\right)$ for every $(\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{C}) \in \mathrm{Lin}$, so that the fourth order tensor $\boldsymbol{I} \boxdot \boldsymbol{I}$ is the symmetrizing operator which associates every second order tensor to its symmetric part.

An immediate consequence of the above definitions is that

$$\mathbb{P}_{\rm P}[\boldsymbol{a} \otimes \boldsymbol{m}] = \mathbb{P}_{\rm P}[\boldsymbol{m} \otimes \boldsymbol{a}] = 0, \tag{18}$$

where $\boldsymbol{a}$ is an arbitrary vector. Moreover, for every symmetric second order tensor $\boldsymbol{A}$, we have that

$$\boldsymbol{A}_{\rm P}\boldsymbol{m} = 0, \tag{19}$$

which, accordingly, implies that

$$\boldsymbol{A}\boldsymbol{m} = 0 \quad \Longleftrightarrow \quad \boldsymbol{A}_{\rm A} = 0. \tag{20}$$

Let us define a rectangular volume V that spans exactly one period along the $\boldsymbol{p}$-direction so that $V = L\ell$, where the length ℓ along the $\boldsymbol{m}$-direction is arbitrary, see Fig. 3. In our analysis it is sufficient to consider that the volume V either contains fully the dislocation dipole ($V = V_{\rm d}$ and $\ell = \ell''$) or is free of defects ($V = V_0$ and $\ell = \ell'$), see Fig. 3. In either case, the boundary of V is defined as $\partial V \equiv \partial V_A \cap \partial V_B \cap \partial V_C \cap \partial V_D$, where ∂V_A, ∂V_B, ∂V_C, and ∂V_D are the planar parts of the boundary ∂V characterized by the outward normals $-\boldsymbol{m}$, $\boldsymbol{p}$, $\boldsymbol{m}$, and $-\boldsymbol{p}$, respectively.

In what follows, we will show that the traction boundary conditions (11) together with the periodicity conditions (12) imply two important properties of the average stress $\bar{\boldsymbol{\sigma}}$ and average strain $\bar{\boldsymbol{\varepsilon}}$ in an arbitrary volume V of the type defined above, viz.

$$\bar{\boldsymbol{\sigma}}_{\rm A} = 0 \quad \text{and} \quad \bar{\boldsymbol{\varepsilon}}_{\rm P} = 0 \quad \text{for any } V. \tag{21}$$

To prove $(21)_1$, we start from the balance of linear momentum for the volume V, namely

$$\int_{\partial V} \boldsymbol{t}^{(\boldsymbol{n})} \mathrm{d}S = 0, \tag{22}$$

where $\boldsymbol{n}$ is the outward unit normal to ∂V. Then, upon integrating explicitly along the boundary of V, Eq. (22) takes the following form

$$\int_{\partial V_A} \boldsymbol{t}^{(-\boldsymbol{m})} \mathrm{d}S + \int_{\partial V_B} \boldsymbol{t}^{(\boldsymbol{p})} \mathrm{d}S + \int_{\partial V_C} \boldsymbol{t}^{(\boldsymbol{m})} \mathrm{d}S + \int_{\partial V_D} \boldsymbol{t}^{(-\boldsymbol{p})} \mathrm{d}S = \boldsymbol{0}. \tag{23}$$

Further, taking into account the periodicity condition $(12)_2$ and the identity $\boldsymbol{t}^{(-\boldsymbol{m})} = -\boldsymbol{t}^{(\boldsymbol{m})}$, Eq. (23) becomes

$$\int_{\partial V_A} \boldsymbol{t}^{(\boldsymbol{m})} \mathrm{d}S = \int_{\partial V_C} \boldsymbol{t}^{(\boldsymbol{m})} \mathrm{d}S. \tag{24}$$

In view of (11), the stress $\boldsymbol{\sigma}$ and consequently the traction $\boldsymbol{t}^{(m)}$ vanish for $\boldsymbol{x} \cdot \boldsymbol{m} \to \pm\infty$. Thus, considering that the volume V can be taken arbitrarily large with the boundary

∂V_A or ∂V_C located at $\boldsymbol{x}\cdot\boldsymbol{m}\to\pm\infty$, the equilibrium condition expressed by (24) implies that the traction $\boldsymbol{t}^{(\boldsymbol{m})}$ vanishes when averaged over ∂V_A or ∂V_C, or any planar surface S_L (Fig. 3) with a normal vector $\boldsymbol{m}$ and length L along $\boldsymbol{p}$,

$$\int_{\partial V_A} \boldsymbol{t}^{(\boldsymbol{m})}\mathrm{d}S = \int_{\partial V_C} \boldsymbol{t}^{(\boldsymbol{m})}\mathrm{d}S = \int_{S_L} \boldsymbol{t}^{(\boldsymbol{m})}\mathrm{d}S = \mathbf{0}. \tag{25}$$

In view of the above, we can write

$$\int_{S_L} \boldsymbol{t}^{(\boldsymbol{m})}\mathrm{d}S = \int_{S_L} \boldsymbol{\sigma}\boldsymbol{m}\,\mathrm{d}S = \left(\int_{S_L} \boldsymbol{\sigma}\mathrm{d}S\right)\boldsymbol{m} = \mathbf{0}, \tag{26}$$

which, in turn, implies that the product of $\boldsymbol{m}$ with the volume integral over V of the stress $\boldsymbol{\sigma}$ is also equal to zero, thus

$$\left(\frac{1}{V}\int_V \boldsymbol{\sigma}\mathrm{d}V\right)\boldsymbol{m} = \mathbf{0}. \tag{27}$$

Consequently, employing the definition of the average stress in $(6)_1$, we have

$$\bar{\boldsymbol{\sigma}}\boldsymbol{m} = \mathbf{0}, \tag{28}$$

which, according to (20), shows that $\bar{\boldsymbol{\sigma}}_\mathrm{A} = 0$ in every V and thus verifies the property $(21)_1$.

Next, we prove the second property, Eq. $(21)_2$. By using the definition $(6)_2$ of the average strain in conjunction with $(15)_1$, $\bar{\boldsymbol{\varepsilon}}_\mathrm{P}$ can be written as

$$\bar{\boldsymbol{\varepsilon}}_\mathrm{P} = \mathbb{P}_\mathrm{P}[\bar{\boldsymbol{\varepsilon}}] = \mathbb{P}_\mathrm{P}\left[\frac{1}{2V}\int_{\partial V}(\boldsymbol{u}\otimes\boldsymbol{n}+\boldsymbol{n}\otimes\boldsymbol{u})\,\mathrm{d}S\right] = \frac{1}{V}\int_{\partial V}\mathbb{P}_\mathrm{P}[\boldsymbol{u}\otimes\boldsymbol{n}]\mathrm{d}V. \tag{29}$$

Then, by integrating explicitly along the boundary ∂V, we obtain

$$\begin{aligned}\bar{\boldsymbol{\varepsilon}}_\mathrm{P} \;=\; & -\frac{1}{V}\int_{\partial V_A}\mathbb{P}_\mathrm{P}[\boldsymbol{u}\otimes\boldsymbol{m}]\mathrm{d}S + \frac{1}{V}\int_{\partial V_B}\mathbb{P}_\mathrm{P}[\boldsymbol{u}\otimes\boldsymbol{p}]\mathrm{d}S \\ & +\frac{1}{V}\int_{\partial V_C}\mathbb{P}_\mathrm{P}[\boldsymbol{u}\otimes\boldsymbol{m}]\mathrm{d}S - \frac{1}{V}\int_{\partial V_D}\mathbb{P}_\mathrm{P}[\boldsymbol{u}\otimes\boldsymbol{p}]\mathrm{d}S,\end{aligned} \tag{30}$$

which by taking into account (18) becomes

$$\bar{\boldsymbol{\varepsilon}}_\mathrm{P} = \frac{1}{V}\mathbb{P}_\mathrm{P}\left[\left(\int_{\partial V_B}\boldsymbol{u}\,dS - \int_{\partial V_D}\boldsymbol{u}\,dS\right)\otimes\boldsymbol{p}\right] = \mathbf{0}, \tag{31}$$

where the term in the paranthesis is equal to zero due to the periodicity condition $(12)_1$. Consequently, $\bar{\boldsymbol{\varepsilon}}_\mathrm{P} = 0$ for every volume V, which verifies Eq. $(21)_2$.

For future use, we introduce also the interior and exterior parts of the average plastic strain $\bar{\boldsymbol{\varepsilon}}^\mathrm{p}$ in the volume V_d. From (8) and with $N=1$, we have

$$\bar{\boldsymbol{\varepsilon}}^\mathrm{p} = \frac{d}{2V}(\boldsymbol{b}\otimes\boldsymbol{\nu}+\boldsymbol{\nu}\otimes\boldsymbol{b}) \quad \text{in } V_\mathrm{d}, \tag{32}$$

and the corresponding interior and exterior parts are found in the form

$$\bar{\varepsilon}^{\mathrm{p}}_{\mathrm{P}} = \frac{d(\boldsymbol{\nu}\cdot\boldsymbol{p})}{V}\left\{(\boldsymbol{b}\cdot\boldsymbol{p})\,\boldsymbol{p}\otimes\boldsymbol{p} + \frac{1}{2}\,(\boldsymbol{b}\cdot\boldsymbol{r})\,(\boldsymbol{p}\otimes\boldsymbol{r}+\boldsymbol{r}\otimes\boldsymbol{p})\right\}, \tag{33}$$

$$\begin{aligned}\bar{\varepsilon}^{\mathrm{p}}_{\mathrm{A}} &= \frac{d(\boldsymbol{\nu}\cdot\boldsymbol{m})}{V}\left\{(\boldsymbol{b}\cdot\boldsymbol{m})\,\boldsymbol{m}\otimes\boldsymbol{m} + \frac{1}{2}\,(\boldsymbol{b}\cdot\boldsymbol{r})\,(\boldsymbol{m}\otimes\boldsymbol{r}+\boldsymbol{r}\otimes\boldsymbol{m})\right\} \\ &\quad + \frac{d}{2V}\{\,(\boldsymbol{b}\cdot\boldsymbol{m})\,(\boldsymbol{\nu}\cdot\boldsymbol{p}) + (\boldsymbol{b}\cdot\boldsymbol{p})\,(\boldsymbol{\nu}\cdot\boldsymbol{m})\,\}\,(\boldsymbol{m}\otimes\boldsymbol{p}+\boldsymbol{p}\otimes\boldsymbol{m})\,.\end{aligned} \tag{34}$$

Obviously, the average plastic strain of a defect-free volume V_0 is equal to zero,

$$\bar{\varepsilon}^{\mathrm{p}} = \mathbf{0} \quad \text{in } V_0. \tag{35}$$

3.3 Mixed form of constitutive equation

It is convenient for the subsequent derivations to introduce an intrinsic coordinate system with its axes parallel to the unit vectors $\boldsymbol{p}$, $\boldsymbol{m}$ and $\boldsymbol{r}$. In this system, the interior-exterior decomposition can be easily expressed componentwise. In particular, using the Kelvin notation, the stress tensor (and similarly the strain tensor) is represented by a vector $\boldsymbol{\sigma}$ in a six-dimensional space, and its interior and exterior parts are represented by three-component subvectors $\boldsymbol{\sigma}_{\mathrm{P}}$ and $\boldsymbol{\sigma}_{\mathrm{A}}$,

$$\boldsymbol{\sigma} = \{\boldsymbol{\sigma}_{\mathrm{P}}, \boldsymbol{\sigma}_{\mathrm{A}}\}, \quad \boldsymbol{\sigma}_{\mathrm{P}} = \{\sigma_{pp}, \sigma_{rr}, \sqrt{2}\sigma_{pr}\}, \quad \boldsymbol{\sigma}_{\mathrm{A}} = \{\sigma_{mm}, \sqrt{2}\sigma_{mr}, \sqrt{2}\sigma_{pm}\}, \tag{36}$$

where $\sigma_{pp} = \boldsymbol{p}\cdot\boldsymbol{\sigma}\boldsymbol{p}$, $\sigma_{pr} = \boldsymbol{p}\cdot\boldsymbol{\sigma}\boldsymbol{r}$, etc. The constitutive equation (9) is then rewritten accordingly,

$$\begin{Bmatrix}\bar{\boldsymbol{\sigma}}_{\mathrm{P}}\\ \bar{\boldsymbol{\sigma}}_{\mathrm{A}}\end{Bmatrix} = \begin{bmatrix}\mathbb{L}_{\mathrm{PP}} & \mathbb{L}_{\mathrm{PA}}\\ \mathbb{L}^{T}_{\mathrm{PA}} & \mathbb{L}_{\mathrm{AA}}\end{bmatrix}\begin{Bmatrix}\bar{\varepsilon}_{\mathrm{P}} - \bar{\varepsilon}^{\mathrm{p}}_{\mathrm{P}}\\ \bar{\varepsilon}_{\mathrm{A}} - \bar{\varepsilon}^{\mathrm{p}}_{\mathrm{A}}\end{Bmatrix}, \tag{37}$$

where $\mathbb{L}_{\mathrm{PP}}$, $\mathbb{L}_{\mathrm{AA}}$, and $\mathbb{L}_{\mathrm{PA}}$ are $3{\times}3$ submatrices of the $6{\times}6$ elasticity matrix $\mathbb{L}$ with its rows and columns adequately rearranged to match (36).

The partial inversion of (37) gives the following *mixed* form of the constitutive equation [23, 24],

$$\begin{Bmatrix}\bar{\boldsymbol{\sigma}}_{\mathrm{P}}\\ \bar{\varepsilon}_{\mathrm{A}} - \bar{\varepsilon}^{\mathrm{p}}_{\mathrm{A}}\end{Bmatrix} = \begin{bmatrix}\mathbb{L}_{\mathrm{PP}} - \mathbb{L}_{\mathrm{PA}}\mathbb{L}^{-1}_{\mathrm{AA}}\mathbb{L}^{T}_{\mathrm{PA}} & \mathbb{L}_{\mathrm{PA}}\mathbb{L}^{-1}_{\mathrm{AA}}\\ -\mathbb{L}^{-1}_{\mathrm{AA}}\mathbb{L}^{T}_{\mathrm{PA}} & \mathbb{L}^{-1}_{\mathrm{AA}}\end{bmatrix}\begin{Bmatrix}\bar{\varepsilon}_{\mathrm{P}} - \bar{\varepsilon}^{\mathrm{p}}_{\mathrm{P}}\\ \bar{\boldsymbol{\sigma}}_{\mathrm{A}}\end{Bmatrix}, \tag{38}$$

which taking into account (21) furnishes

$$\begin{Bmatrix}\bar{\boldsymbol{\sigma}}_{\mathrm{P}}\\ \bar{\varepsilon}_{\mathrm{A}} - \bar{\varepsilon}^{\mathrm{p}}_{\mathrm{A}}\end{Bmatrix} = \begin{bmatrix}\mathbb{L}_{\mathrm{PP}} - \mathbb{L}_{\mathrm{PA}}\mathbb{L}^{-1}_{\mathrm{AA}}\mathbb{L}^{T}_{\mathrm{PA}} & \mathbb{L}_{\mathrm{PA}}\mathbb{L}^{-1}_{\mathrm{AA}}\\ -\mathbb{L}^{-1}_{\mathrm{AA}}\mathbb{L}^{T}_{\mathrm{PA}} & \mathbb{L}^{-1}_{\mathrm{AA}}\end{bmatrix}\begin{Bmatrix}-\bar{\varepsilon}^{\mathrm{p}}_{\mathrm{P}}\\ \mathbf{0}\end{Bmatrix}. \tag{39}$$

It is noted that positive definiteness of $\mathbb{L}$ guarantees that $\mathbb{L}_{\mathrm{AA}}$ is also positive definite, which, in turn, implies that it can be inverted. The mixed form (39) has been conveniently obtained in the intrinsic coordinate system using the Kelvin matrix notation and the corresponding interior-exterior decomposition. In the subsequent sections, the use of the

Kelvin matrix notation will be explicitly stated, otherwise the standard tensorial notation is employed.

It is seen from (39) that a nonzero average stress $\bar{\boldsymbol{\sigma}}_{\mathrm{P}}$ is associated with a nonzero interior part $\bar{\boldsymbol{\varepsilon}}^{\mathrm{p}}_{\mathrm{P}}$ of the average plastic strain $\bar{\boldsymbol{\varepsilon}}^{\mathrm{p}}$. If the volume contains the dislocation dipole, i.e. for $V = V_{\mathrm{d}}$, then the interior part $\bar{\boldsymbol{\varepsilon}}^{\mathrm{p}}_{\mathrm{P}}$ of the average plastic strain is given by (33), and the possibly nonzero components $\bar{\boldsymbol{\sigma}}_{\mathrm{P}}$ and $\bar{\boldsymbol{\varepsilon}}_{\mathrm{A}}$ are given by (39) in conjunction with (34), for arbitrary anisotropy of the material. On the other hand, for a defect-free volume, i.e. for $V = V_0$, the average plastic strain is equal to zero. Accordingly, Eq. (35), when combined with (21), yields

$$\bar{\boldsymbol{\sigma}} = \mathbf{0} \quad \text{and} \quad \bar{\boldsymbol{\varepsilon}} = \mathbf{0} \quad \text{in } V_0. \tag{40}$$

4 Doubly periodic array of dislocation dipoles

The material is now assumed to be composed of a doubly periodic array of dislocation dipoles (Fig. 4). Such a configuration can be obtained by taking the string of dipoles defined by vector $\boldsymbol{p}$ and spacing L_1 and by superposing its replicas in the normal direction $\boldsymbol{m}$ with spacing L_2. The corresponding stress field is thus given by, cf. Eq. (10),

$$\boldsymbol{\sigma}(\boldsymbol{x}) = \sum_{j=-\infty}^{+\infty} \sum_{i=-\infty}^{+\infty} \left[\boldsymbol{\sigma}_{\boldsymbol{b}}(\boldsymbol{x} - \boldsymbol{x}^{+} - iL_1\boldsymbol{p} - jL_2\boldsymbol{m}) - \boldsymbol{\sigma}_{\boldsymbol{b}}(\boldsymbol{x} - \boldsymbol{x}^{-} - iL_1\boldsymbol{p} - jL_2\boldsymbol{m})\right]. \tag{41}$$

Considering that the stress field of a single string of dislocation dipoles decays exponentially in the direction normal to the string [19], it is usually sufficient to include just a few terms in the outer summation. Again, we stress that the knowledge of the local fields, e.g., the local stress field (41), is not needed for the subsequent analysis.

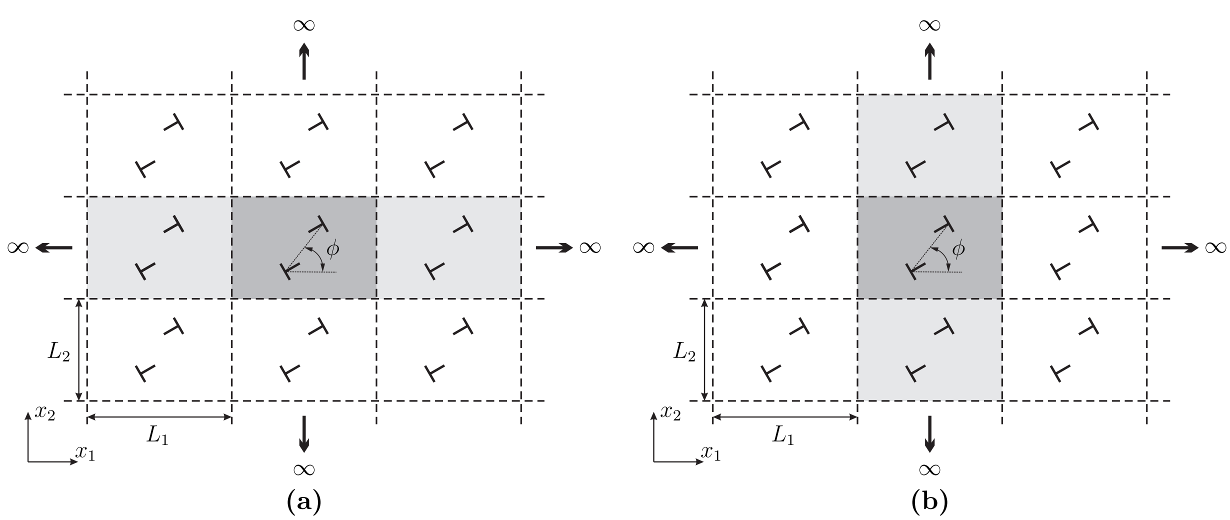

Figure 4: Doubly periodic array of dislocation dipoles: construction by superposition of (a) horizontal strings and (b) vertical strings. The primary strings employed in the superposition schemes are depicted in grey.

While the summation scheme (41) is needed to compute the local stress field, we notice that, in view of (40), the *average* stress and strain associated with arbitrary volumes V_d and V_0, such as those defined in Fig. 3, are actually not affected by the neighboring strings. In particular, this means that the average stress and strain determined for the doubly periodic array of dipoles for the volume $V = L_1 L_2$ of the periodic cell are equal to the respective average quantities determined for the single string of dislocation dipoles for the adequate volume V_d.

For the doubly periodic array of dislocation dipoles, the average stress and strain associated with the volume $V = L_1 L_2$ of the periodic cell are naturally identified as the *macroscopic* stress and strain.

$$\boldsymbol{\Sigma} = \bar{\boldsymbol{\sigma}}, \qquad \boldsymbol{E} = \bar{\boldsymbol{\varepsilon}}, \qquad \boldsymbol{E}^\mathrm{p} = \bar{\boldsymbol{\varepsilon}}^\mathrm{p}, \tag{42}$$

which, in view of (9) and (32), satisfy the macroscopic constitutive equation

$$\boldsymbol{\Sigma} = \mathbb{L}[\boldsymbol{E} - \boldsymbol{E}^\mathrm{p}] \qquad \text{with} \quad \boldsymbol{E}^\mathrm{p} = \frac{d}{2V}(\boldsymbol{b} \otimes \boldsymbol{\nu} + \boldsymbol{\nu} \otimes \boldsymbol{b}), \tag{43}$$

According to (21), we immediately have

$$\boldsymbol{\Sigma}_\mathrm{A} = 0 \quad \text{and} \quad \boldsymbol{E}_\mathrm{P} = 0, \tag{44}$$

so that $\boldsymbol{\Sigma} = \boldsymbol{\Sigma}_\mathrm{P}$ and $\boldsymbol{E} = \boldsymbol{E}_\mathrm{A}$, where the exterior and interior parts are defined with respect to the vector $\boldsymbol{m}$ that is normal to the primary string of dipoles that was superposed in order to construct the doubly periodic configuration. Furthermore, the interior $\boldsymbol{E}^\mathrm{p}_\mathrm{P}$ and exterior $\boldsymbol{E}^\mathrm{p}_\mathrm{A}$ parts of the macroscopic plastic strain $\boldsymbol{E}^\mathrm{p}$ are given by (33) and (34), respectively. Finally, the yet unknown components $\boldsymbol{\Sigma}_\mathrm{P}$ and $\boldsymbol{E}_\mathrm{A}$ follow from the constitutive equation in the mixed form (39) formulated in terms of the macroscopic quantities $\boldsymbol{\Sigma}$ and $\boldsymbol{E}$. Specifically, in the Kelvin matrix notation introduced in Section 3.3, we have

$$\boldsymbol{\Sigma}_\mathrm{P} = -\left(\mathbb{L}_\mathrm{PP} - \mathbb{L}_\mathrm{PA}\mathbb{L}^{-1}_\mathrm{AA}\mathbb{L}^T_\mathrm{PA}\right)\boldsymbol{E}^\mathrm{p}_\mathrm{P}, \qquad \boldsymbol{E}^\mathrm{e}_\mathrm{A} = \boldsymbol{E}_\mathrm{A} - \boldsymbol{E}^\mathrm{p}_\mathrm{A} = \mathbb{L}^{-1}_\mathrm{AA}\mathbb{L}^T_\mathrm{PA}\boldsymbol{E}^\mathrm{p}_\mathrm{P}. \tag{45}$$

It is remarked that the macroscopic stress $\boldsymbol{\Sigma} = \boldsymbol{\Sigma}_\mathrm{P}$ depends, through $\boldsymbol{E}^\mathrm{p}_\mathrm{P}$ and submatrices $\mathbb{L}_{\alpha\beta}$, on the summation scheme adopted while constructing the doubly periodic array of dislocation dipoles. That macroscopic stress is *exactly* the spurious stress associated with the conditional convergence of the lattice sums in a general anisotropic material, and the corresponding formula $(45)_1$ constitutes the main result of the present work. We also point out that, contrary to the approach of Kuykendall and Cai [20], the spurious macroscopic stress is derived here without using the analytical solutions for individual dislocations.

Equations (45) have been obtained for the case of the unit cell containing one dislocation dipole. The formulae for the case of several dipoles are identical, with the macroscopic plastic strain $\boldsymbol{E}^\mathrm{p}$ being now the sum of contributions of individual dipoles, as in (8). The case of an arbitrary arrangement of dislocations of the total net Burgers vector equal to zero can be treated by constructing an equivalent ensemble of dislocation dipoles.

Now, referring to a fixed Cartesian system with the basis $\boldsymbol{e}_i$, we examine two common summation schemes employed for the construction of a doubly periodic array of dipoles, cf. Fig. 4. In this coordinate system, the orientation of the dislocation dipole with respect to the x_1-axis is characterized by angle ϕ, which obviously does not depend on the adopted summation scheme.

Case I: Superposition of horizontal strings of dislocation dipoles The doubly periodic array is now constructed by the superposition of *horizontal* strings of dislocation dipoles along the x_2-direction. We have thus $\boldsymbol{p} = \boldsymbol{e}_1$, $\boldsymbol{m} = \boldsymbol{e}_2$ and $\boldsymbol{r} = \boldsymbol{e}_3$, so that $\boldsymbol{b}\cdot\boldsymbol{p} = b_1$, $\boldsymbol{b}\cdot\boldsymbol{r} = b_3$, $\boldsymbol{\nu}\cdot\boldsymbol{p} = -\sin\phi$, and

$$\boldsymbol{E}_{\mathrm{P}}^{\mathrm{p}} = -\frac{d\sin\phi}{V}\left(b_1\boldsymbol{e}_1\otimes\boldsymbol{e}_1 + \frac{b_3}{2}\left(\boldsymbol{e}_1\otimes\boldsymbol{e}_3 + \boldsymbol{e}_3\otimes\boldsymbol{e}_1\right)\right), \tag{46}$$

or, equivalently, in terms of the components of $\boldsymbol{E}_{\mathrm{P}}^{\mathrm{p}}$,

$$E_{11}^{\mathrm{p}} = -\frac{b_1\Delta x_2}{L_1L_2}, \quad E_{13}^{\mathrm{p}} = -\frac{b_3\Delta x_2}{2L_1L_2}, \quad E_{33}^{\mathrm{p}} = 0, \tag{47}$$

where $\Delta x_2 = d\sin\phi$ is the vertical distance between the dislocations forming the dipole in the periodic cell. Note that for $\phi = 0$ (i.e., for $\Delta x_2 = 0$) we have $\boldsymbol{E}_{\mathrm{P}}^{\mathrm{p}} = \boldsymbol{0}$, which, according to $(45)_1$, implies that no spurious stresses are produced in the doubly periodic array by this summation scheme. Finally, we remark that the components of $\boldsymbol{\Sigma}_{\mathrm{P}}$ and $\boldsymbol{E}_{\mathrm{A}}$ in the Kelvin matrix notation are

$$\boldsymbol{\Sigma}_{\mathrm{P}} = \{\Sigma_{11}, \Sigma_{33}, \sqrt{2}\Sigma_{13}\}, \quad \boldsymbol{E}_{\mathrm{A}} = \{E_{22}, \sqrt{2}E_{23}, \sqrt{2}E_{12}\}, \tag{48}$$

while, obviously, $\boldsymbol{\Sigma}_{\mathrm{A}} = \boldsymbol{0}$ and $\boldsymbol{E}_{\mathrm{P}} = \boldsymbol{0}$.

Case II: Superposition of vertical strings of dislocation dipoles In this case, the doubly periodic array is constructed by the superposition of *vertical* strings of dislocation dipoles along the x_1-direction. We have now $\boldsymbol{p} = \boldsymbol{e}_2$, $\boldsymbol{m} = -\boldsymbol{e}_1$, and $\boldsymbol{r} = \boldsymbol{e}_3$. Consequently, $\boldsymbol{b}\cdot\boldsymbol{p} = b_2$, $\boldsymbol{b}\cdot\boldsymbol{r} = b_3$, $\boldsymbol{\nu}\cdot\boldsymbol{p} = \cos\phi$, and

$$\boldsymbol{E}_{\mathrm{P}}^{\mathrm{p}} = \frac{d\cos\phi}{V}\left(b_2\boldsymbol{e}_2\otimes\boldsymbol{e}_2 + \frac{b_3}{2}\left(\boldsymbol{e}_2\otimes\boldsymbol{e}_3 + \boldsymbol{e}_3\otimes\boldsymbol{e}_2\right)\right), \tag{49}$$

and in terms of the components of $\boldsymbol{E}_{\mathrm{P}}^{\mathrm{p}}$,

$$E_{22}^{\mathrm{p}} = \frac{b_2\Delta x_1}{L_1L_2}, \quad E_{23}^{\mathrm{p}} = \frac{b_3\Delta x_1}{2L_1L_2}, \quad E_{33}^{\mathrm{p}} = 0, \tag{50}$$

where $\Delta x_1 = d\cos\phi$ is the horizontal distance between the dislocations in the periodic cell. In this case, $\boldsymbol{E}_{\mathrm{P}}^{\mathrm{p}}$ and accordingly the spurious stresses vanish when $\phi = \pm\pi/2$ (i.e., when $\Delta x_1 = 0$). The components of $\boldsymbol{\Sigma}_{\mathrm{P}}$ and $\boldsymbol{E}_{\mathrm{A}}$ in the Kelvin matrix notation are now

$$\boldsymbol{\Sigma}_{\mathrm{P}} = \{\Sigma_{22}, \Sigma_{33}, \sqrt{2}\Sigma_{23}\}, \quad \boldsymbol{E}_{\mathrm{A}} = \{E_{11}, -\sqrt{2}E_{13}, -\sqrt{2}E_{12}\}, \tag{51}$$

where the minus signs appear as a result of the definitions adopted in (36).

4.1 Isotropic material

Elastic properties are now specified by the shear modulus μ and the Poisson's ratio ν. Taking into account (45) in conjunction with (47) and (50), we obtain explicit formulae for the components of $\boldsymbol{\Sigma}_{\mathrm{P}}$ and $\boldsymbol{E}^{\mathrm{e}}_{\mathrm{A}}$ corresponding to the two summation schemes. The remaining components of $\boldsymbol{\Sigma}$, $\boldsymbol{E}$ and $\boldsymbol{E}^{\mathrm{e}}$ are trivially obtained from the relationships: $\boldsymbol{\Sigma}_{\mathrm{A}} = \mathbf{0}$, $\boldsymbol{E}_{\mathrm{P}} = \mathbf{0}$ and $\boldsymbol{E} = \boldsymbol{E}^{\mathrm{e}} + \boldsymbol{E}^{\mathrm{p}}$.

It is noted that the formulae for the components of the macroscopic stress given below in (52) and (54) are equivalent to the respective formulae for the constant spurious stresses derived previously by Kuykendall and Cai [20] using a different procedure.

Case I: Superposition of horizontal strings of dislocation dipoles

$$\Sigma_{11} = \frac{2\mu b_1 \Delta x_2}{(1-\nu)\, L_1 L_2}, \quad \Sigma_{13} = \frac{\mu b_3 \Delta x_2}{L_1 L_2}, \quad \Sigma_{33} = \nu \Sigma_{11}, \quad \Sigma_{22} = \Sigma_{23} = \Sigma_{12} = 0, \tag{52}$$

$$\begin{aligned} E^{\mathrm{e}}_{22} &= -\frac{\nu b_1 \Delta x_2}{(1-\nu)\, L_1 L_2}, \quad E^{\mathrm{e}}_{23} = E^{\mathrm{e}}_{12} = 0, \\ E^{\mathrm{e}}_{11} &= -E^{\mathrm{p}}_{11}, \quad E^{\mathrm{e}}_{13} = -E^{\mathrm{p}}_{13}, \quad E^{\mathrm{e}}_{33} = 0. \end{aligned} \tag{53}$$

Case II: Superposition of vertical strings of dislocation dipoles

$$\Sigma_{22} = -\frac{2\mu b_2 \Delta x_1}{(1-\nu)\, L_1 L_2}, \quad \Sigma_{23} = -\frac{\mu b_3 \Delta x_1}{L_1 L_2}, \quad \Sigma_{33} = \nu \Sigma_{22}, \quad \Sigma_{11} = \Sigma_{13} = \Sigma_{12} = 0, \tag{54}$$

$$\begin{aligned} E^{\mathrm{e}}_{11} &= \frac{\nu b_2 \Delta x_1}{(1-\nu)\, L_1 L_2}, \quad E^{\mathrm{e}}_{13} = E^{\mathrm{e}}_{12} = 0, \\ E^{\mathrm{e}}_{22} &= -E^{\mathrm{p}}_{22}, \quad E^{\mathrm{e}}_{23} = -E^{\mathrm{p}}_{23}, \quad E^{\mathrm{e}}_{33} = 0. \end{aligned} \tag{55}$$

4.2 Orthotropic material

For an orthotropic material, the elastic properties are specified by nine elastic constants c_{ij} [25]. We consider a special orientation of the doubly periodic array of dipoles with respect to the orthotropy axes, namely we assume that the principal axes of orthotropy are aligned with the vectors $\boldsymbol{e}_1$, $\boldsymbol{e}_2$ and $\boldsymbol{e}_3$, respectively. This special orientation is taken here as an example, to illustrate the applicability of the general formulae (45), and no reference is made to any physically relevant orientation of crystalline lattice and crystallographic slip systems. The macroscopic spurious stresses and the respective elastic strains corresponding to the two summation schemes are given below. Clearly, the formulae for transversal isotropy and cubic symmetry are obtained as special cases of the formulae provided below.

Case I: Superposition of horizontal strings of dislocation dipoles

$$\Sigma_{11} = \frac{(c_{11}c_{22} - c_{12}^2)\, b_1 \Delta x_2}{c_{22} L_1 L_2}, \quad \Sigma_{13} = \frac{c_{55} b_3 \Delta x_2}{2 L_1 L_2}, \quad \Sigma_{33} = \frac{(c_{22}c_{13} - c_{12}c_{23})\, b_1 \Delta x_2}{c_{22} L_1 L_2},$$

$$\Sigma_{11} = 0, \quad \Sigma_{13} = 0 \quad \Sigma_{12} = 0, \tag{56}$$

and

$$E^{\mathrm{e}}_{22} = -\frac{c_{12} b_1 \Delta x_2}{c_{22} L_1 L_2}, \quad E^{\mathrm{e}}_{23} = 0, \quad E^{\mathrm{e}}_{12} = 0,$$

$$E^{\mathrm{e}}_{11} = -E^{\mathrm{p}}_{11}, \quad E^{\mathrm{e}}_{13} = -E^{\mathrm{p}}_{13}, \quad E^{\mathrm{e}}_{33} = 0. \tag{57}$$

Case II: Superposition of vertical strings of dislocation dipoles

$$\Sigma_{22} = -\frac{(c_{11}c_{22} - c_{12}^2)\, b_2 \Delta x_1}{c_{11} L_1 L_2}, \quad \Sigma_{23} = -\frac{c_{44} b_3 \Delta x_1}{2 L_1 L_2}, \quad \Sigma_{33} = -\frac{(c_{11}c_{23} - c_{12}c_{13})\, b_2 \Delta x_1}{c_{11} L_1 L_2},$$

$$\Sigma_{11} = 0, \quad \Sigma_{13} = 0, \quad \Sigma_{12} = 0, \tag{58}$$

and

$$E^{\mathrm{e}}_{11} = \frac{c_{12} b_2 \Delta x_1}{c_{11} L_1 L_2}, \quad E^{\mathrm{e}}_{13} = 0, \quad E^{\mathrm{e}}_{12} = 0,$$

$$E^{\mathrm{e}}_{22} = -E^{\mathrm{p}}_{22}, \quad E^{\mathrm{e}}_{23} = -E^{\mathrm{p}}_{23}, \quad E^{\mathrm{e}}_{33} = 0. \tag{59}$$

5 Macroscopic stress determined from the Eshelby's solution

So far we have considered two summation schemes, and we have shown that the conditional convergence resulting in spurious macroscopic stresses is related to the conditions enforced on the far-field stresses. Specifically, for a single string of dislocation dipoles, the stress vanishes far from the string but not necessarily along the string.

One may consider another summation scheme in which the stress field in the primary cell is obtained as a superposition of the stress fields of the dipoles contained within a circle of radius R, Fig. 5. In that case, the stress vanishes far from the primary cell in all directions, i.e., for $r \to \infty$, r being the distance from the centre of the primary cell. With increasing truncation radius R, the stress field is expected to converge, but it is also expected to contain a spurious stress in view of the conditional convergence of the infinite summation (41).

Now, considering a homogenized medium governed by the macroscopic constitutive equation $\boldsymbol{\Sigma} = \mathbb{L}[\boldsymbol{E} - \boldsymbol{E}^{\mathrm{p}}]$, Eq. $(43)_1$, i.e., neglecting the stress fluctuations within the individual cells, the present summation scheme is immediately recognized to correspond to the Eshelby problem of a circular inclusion in an elastic matrix. The uniform stress within the inclusion is then given by the classical formula [21]

$$\boldsymbol{\Sigma} = \mathbb{L}(\mathbb{S} - \mathbb{I})[\boldsymbol{E}^{\mathrm{p}}], \tag{60}$$

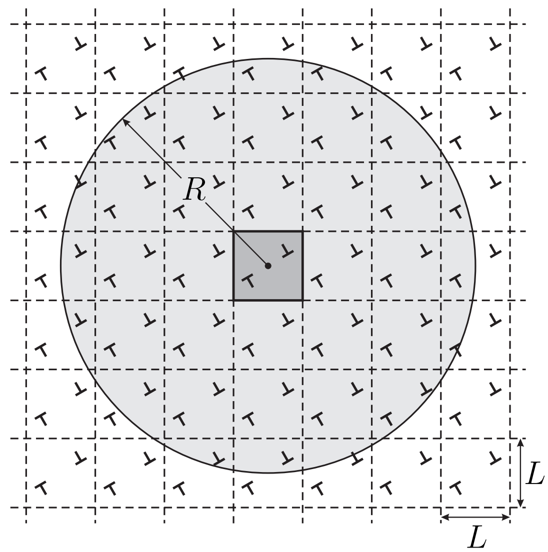

Figure 5: Circular summation scheme.

where $\mathbb{S}$ is the Eshelby tensor, $\mathbb{I}$ is the fourth-order unity tensor, and the macroscopic plastic strain $\boldsymbol{E}^{\mathrm{p}}$ given by $(43)_2$ is the uniform eigenstrain of the inclusion.

The problem can actually be formulated for a more general summation scheme in which the summation is performed over an elliptical region with a fixed ratio of the semiaxes a_1 and a_2 so that the summation scheme corresponds to the Eshelby problem for an elliptical inclusion. Confining our attention to the case of elastic *isotropy*, Eq. (60) yields the following formulae, cf. [26], for the components of the macroscopic stress $\boldsymbol{\Sigma}$:

$$\begin{aligned}
\Sigma_{11} &= \frac{\mu}{(1-\nu)} \left\{ \left(-2 + \frac{a_2^2 + 2a_1a_2}{(a_1+a_2)^2} + \frac{a_2}{a_1+a_2} \right) E_{11}^{\mathrm{p}} + \left(\frac{a_2^2}{(a_1+a_2)^2} - \frac{a_2}{a_1+a_2} \right) E_{22}^{\mathrm{p}} \right\}, \\
\Sigma_{22} &= \frac{\mu}{(1-\nu)} \left\{ \left(-2 + \frac{a_1^2 + 2a_1a_2}{(a_1+a_2)^2} + \frac{a_1}{a_1+a_2} \right) E_{22}^{\mathrm{p}} + \left(\frac{a_1^2}{(a_1+a_2)^2} - \frac{a_1}{a_1+a_2} \right) E_{11}^{\mathrm{p}} \right\}, \\
\Sigma_{33} &= -\frac{2\mu\nu}{(1-\nu)(a_1+a_2)} \left(a_1 E_{11}^{\mathrm{p}} + a_2 E_{22}^{\mathrm{p}} \right), \quad \Sigma_{12} = -\frac{2\mu}{(1-\nu)} \frac{a_1a_2}{(a_1+a_2)^2} E_{12}^{\mathrm{p}}, \\
\Sigma_{23} &= -2\mu \frac{a_2}{a_1+a_2} E_{23}^{\mathrm{p}}, \quad \Sigma_{13} = -2\mu \frac{a_1}{a_1+a_2} E_{13}^{\mathrm{p}},
\end{aligned} \tag{61}$$

where the components E_{ij}^{p} of the macroscopic plastic strain $\boldsymbol{E}^{\mathrm{p}}$ are found from $(43)_2$. Notice that in our case $E_{33}^{\mathrm{p}} = 0$.

In the special case of a circular inclusion ($a_1 = a_2$), the formulae for the components of $\boldsymbol{\Sigma}$ take a particularly simple form,

$$\begin{aligned}
\Sigma_{11} &= -\frac{\mu}{4(1-\nu)} \left(3E_{11}^{\mathrm{p}} + E_{22}^{\mathrm{p}} \right), \quad \Sigma_{22} = -\frac{\mu}{4(1-\nu)} \left(E_{11}^{\mathrm{p}} + 3E_{22}^{\mathrm{p}} \right), \\
\Sigma_{33} &= -\frac{\mu\nu}{(1-\nu)} \left(E_{11}^{\mathrm{p}} + E_{22}^{\mathrm{p}} \right), \quad \Sigma_{12} = -\frac{\mu}{2(1-\nu)} E_{12}^{\mathrm{p}}, \\
\Sigma_{23} &= -\mu E_{23}^{\mathrm{p}}, \quad \Sigma_{13} = -\mu E_{13}^{\mathrm{p}}.
\end{aligned} \tag{62}$$

The above stresses are now identified as the spurious stresses that correspond to the circular summation scheme depicted in Fig. 6.

Moreover, it can be easily checked that, in the special case of a plate-like inclusion, i.e., for $a_1 \to \infty$ or $a_2 \to \infty$, the formulae corresponding to the two summation schemes involving superposition of strings of dipoles, see Eqs. (52)–(55) in Section 4.1, are recovered from the general formulae (61).

An application of the formulae (62) corresponding to the circular summation scheme of Fig. 5 is illustrated in Fig. 6. For a fixed truncation radius R, the stress field is evaluated numerically as a superposition of the stress fields of individual dislocation dipoles for which $r \leq R$, where r is the distance from the centre of the current dipole to the centre of the dipole in the primary cell (assumed here to be square). The average stress $\bar{\boldsymbol{\sigma}}$ in the primary cell is then computed, and Fig. 6 shows the components of $\bar{\boldsymbol{\sigma}}$ normalized by the respective components of the macroscopic stress $\bar{\boldsymbol{\Sigma}}$, determined from the Eshelby solution, as a function of the truncation radius R. It is seen that, with increasing R, the average stress $\bar{\boldsymbol{\sigma}}$ indeed converges to the macroscopic stress $\bar{\boldsymbol{\Sigma}}$ predicted by (62).

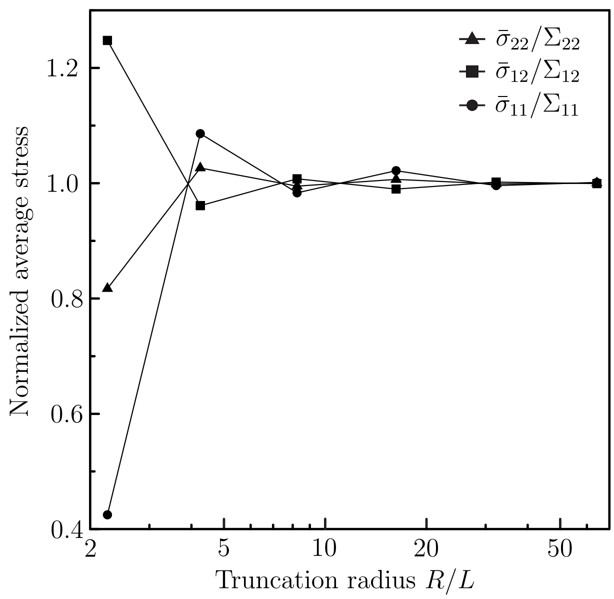

Figure 6: Convergence of the average stress $\bar{\boldsymbol{\sigma}}$ in the primary cell to the macroscopic stress $\boldsymbol{\Sigma}$ determined from the Eshelby solution according to (62). The dipoles are characterized by the Burgers vector $\boldsymbol{b} = (\sqrt{3}b/2, b/2, 0)$, the slip-plane angle $\phi = \pi/6$, and distance $d = L/6$. The Poisson's ratio of the material is $\nu = 1/3$.

6 Conclusions

In this work, we provide a simple physical explanation of the origin of the conditional convergence of lattice sums of image interactions in 2D periodic dislocation arrays. It has been shown that each summation scheme corresponds to specific conditions for the stresses at infinity. Consequently, the stress fields obtained by direct summation of the contributions of individual dislocation dipoles are not pure fluctuations, but also contain a *spurious* macroscopic stress which depends on the conditions imposed by the summation scheme on the far-field stresses. The spurious macroscopic stresses have been determined in a closed form for an arbitrary elastic anisotropy. Importantly, the stress fields of individual dislocations are not needed to derive the corresponding formulae. An alternative procedure has also been developed in which the macroscopic spurious stresses are evaluated employing the Eshelby's solution of an elliptical inclusion in an elastic matrix.

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