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The pair distribution function for an array of screw dislocations

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Abstract

The paper addresses the problem of correlation within an array of parallel dislocations in a crystalline solid. The first two of a hierarchy of equations for the multi-point distribution functions are derived by treating the random dislocation distributions and the corresponding stress fields in an ensemble average framework. Asymptotic reasoning, applicable when dislocations are separated by small distances, provides equations that are independent of any specific kinetic law relating the velocity of a dislocation to the force acting on it. The only assumption made is that the force acting on any dislocation remains finite. The hierarchy is closed by making a standard closure approximation. For the particular case of a population of parallel screw dislocations of the same sign moving on parallel slip planes the solution for the pair distribution function is found analytically. For the dislocations having opposite signs the system of equations suggests that in ensemble average only geometrically necessary dislocations correlate, while balanced positive and negative dislocations would create dipoles or annihilate. Direct numerical simulations support this conclusion. In addition, the relation of the dislocation correlation to strain gradient theories and size effect is shown and discussed.

Keywords: Dislocations; Pair distribution functions; Strain-gradient plasticity

1. Introduction

In a crystalline solid, the interaction of dislocations with the underlying lattice, grain boundaries, inclusions and each other affects their resultant mobility at the microscopic level and, at the macroscopic level, the solid's elastoplastic response to stress. This was recognised even before the existence of dislocations had been experimentally confirmed (Taylor, 1934). Since the 1960's, attempts of varying degrees of sophistication have been made, to identify and eventually to quantify the link between plastic flow and the motion of the associated dislocation structures. At the level of continuous distributions of dislocations, early contributions include those of Mura (1965, 1967) and the mathematically-sophisticated work of Berdichevskii and Sedov (1967). More recent trends have been to set up numerical simulations for a body containing a large number of discrete dislocations (e.g. Van der Giessen et al., 2001). Dislocation arrays have also been treated as random and have

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been subjected to treatments involving ensemble averaging (e.g. Groma, 1997 and succeeding work discussed later). The objective here is to generate and solve equations that govern multipoint probability densities for the locations of the dislocations. In early work, Groma (1997) closed his system of equations at the level of the "mean field approximation" and related this to classical continuum plasticity theory. Subsequent work (e.g. Zaiser et al., 2001, Groma et al., 2003, Zaiser and Aifantis, 2006) admitted the influence of pair distribution functions on dislocation patterning, and in generating equations for continuum plasticity including the effect of gradients of plastic strain. They derived, but did not solve, equations for the two-point functions, obtaining these functions instead from the results of simulations.

The present work follows the line established by Groma (1997). First, a derivation is given for the ensemble averaged descriptions of the dislocation array and the stress that it generates. A hierarchy of equations for the multipoint densities follows once a kinetic law governing the motion of the dislocations is postulated. However, the objective of determining the multipoint densities when the dislocations are close (and so interactions are strong) is served by recognising that equations governing their asymptotic "close" form require only the postulate that the force on any dislocation must be finite. The resulting simplified hierarchy is then closed by a standard closure assumption which neglects the interaction of three dislocations, all close together. The equation governing the two-point probability density for an array of screw dislocations, all of the same sign, all with glide planes parallel to the (x_1, x_3)-plane, is deduced, and a simple analytic solution is presented. When dislocations of either sign are admitted, it is found that the governing equations admit no solution. This paradox is resolved by recognising that dislocations of opposite sign would come into coincidence and either cancel or else form dipoles that would interact only weakly with the remaining free dislocations. Support for this proposition is provided by a simulation, reported here. Finally, reasoning like that of Groma et al. (2003) and Zaiser and Aifantis (2006) is applied to the present system, to develop an explicit correspondence between the present formulation and strain-gradient plasticity. The main difference between this and earlier work is that it is completely analytical and self-contained, the two-point density having been derived from its governing equation.

2. Equations for joint probability densities

The concern here is for an array of straight dislocations, all parallel to the axis Ox_3, in a cylindrical body whose cross-section is a domain $\mathcal{D}$ in the (x_1, x_2)-plane. The possibility that $\mathcal{D}$ could be the whole (x_1, x_2)-plane is included. There could be several types of dislocations, distinguished by a Greek letter index. They are assumed to be distributed randomly at some initial instant. Their motion will follow a deterministic law but their subsequent positions will reflect the initial randomness. The underlying stochastic process is defined in terms of a sample parameter ω which belongs to the sample space Ω over which is defined a probability measure p. Thus, in realization ω the dislocations of type α have positions $\mathbf{x}_i^\alpha(\omega, t)$ at time t, where $i \in I^\alpha$, the index set identifying each individual dislocation of type α. The density of dislocations of type α is defined as follows. Let ϕ be a "test function", infinitely differentiable and having compact support within $\mathcal{D}$. Then

$$\Phi(\omega, t) := \sum_{i \in I^\alpha} \phi(\mathbf{x}_i(\omega, t)) \equiv \sum_{i \in I^\alpha} \int_{\mathcal{D}} \phi(\mathbf{x}) \delta(\mathbf{x} - \mathbf{x}_i^\alpha(\omega, t)) \mathrm{d}\mathbf{x} \tag{2.1}$$

has ensemble mean

$$\langle \Phi \rangle(t) = \int_\Omega p(\mathrm{d}\omega) \Phi(\omega, t). \tag{2.2}$$

This is a linear functional of ϕ and hence can be written

$$\langle \Phi \rangle(t) = \int_{\mathcal{D}} \rho_1^\alpha(\mathbf{x}, t) \phi(\mathbf{x}) \mathrm{d}\mathbf{x}, \tag{2.3}$$

where, formally at least, the distribution $\rho_1^\alpha(\mathbf{x}, t)$ is defined by

$$\rho_1^\alpha(\mathbf{x}, t) = \int_\Omega p(\mathrm{d}\omega) \sum_{i \in I^\alpha} \delta(\mathbf{x} - \mathbf{x}_i^\alpha(\omega, t)). \tag{2.4}$$

Note that the introduction of the test function ϕ ensures that all sums are finite and hence any problems relating to convergence are avoided.

A conservation law for ρ_1^α can now be obtained by calculating $\mathrm{d}\langle\Phi\rangle/\mathrm{d}t$ in two different ways. From (2.2) and (2.1), assuming that no dislocations are created or destroyed (so that I^α is time-independent),

$$\frac{\mathrm{d}\langle\Phi\rangle}{\mathrm{d}t} = \int_\Omega p(\mathrm{d}\omega)\sum_{i\in I^\alpha}\dot{\mathbf{x}}_i^\alpha(\omega,t)\cdot\nabla\phi(\mathbf{x}_i^\alpha(\omega,t)) \equiv \int_{\mathcal{D}}\rho_1^\alpha(\mathbf{x},t)\mathbf{v}^\alpha(\mathbf{x},t)\cdot\nabla\phi(\mathbf{x})\mathrm{d}\mathbf{x}. \tag{2.5}$$

The superposed dot means $\partial/\partial t$. The definition of the velocity field $\mathbf{v}^\alpha(\mathbf{x},t)$ through

$$\int_\Omega p(\mathrm{d}\omega)\sum_{i\in I^\alpha}\dot{\mathbf{x}}_i^\alpha(\omega,t)\psi(\mathbf{x}_i^\alpha(\omega,t)) =: \int_{\mathcal{D}}\rho_1^\alpha(\mathbf{x},t)\mathbf{v}^\alpha(\mathbf{x},t)\psi(\mathbf{x})\mathrm{d}\mathbf{x} \tag{2.6}$$

for any test function ψ is good so long as the density $\rho_1^\alpha(\mathbf{x},t)$ in fact is continuous.

The other expression for $\mathrm{d}\langle\Phi\rangle/\mathrm{d}t$ is obtained from (2.3):

$$\frac{\mathrm{d}\langle\Phi\rangle}{\mathrm{d}t} = \int_{\mathcal{D}}\frac{\partial\rho_1^\alpha}{\partial t}\phi(\mathbf{x})\mathrm{d}\mathbf{x}. \tag{2.7}$$

It follows from (2.5) and (2.7) that

$$\frac{\partial\rho_1^\alpha(\mathbf{x},t)}{\partial t} + \nabla\cdot(\mathbf{v}^\alpha(\mathbf{x},t)\rho_1^\alpha(\mathbf{x},t)) = 0, \tag{2.8}$$

in the sense of distributions. If dislocations were created or destroyed, this would simply introduce a source term on the right side of this equation (see, for instance, Aifantis, 1987).

Multipoint densities can be treated similarly. For two points, and dislocation types α and β, adopt a test function $\phi_2(\mathbf{x},\mathbf{y})$ defined over $\mathcal{D}\times\mathcal{D}$, and let

$$\Phi_2(\omega,t) := \sum_{i\in I^\alpha}\sum_{j\in I^\beta}\phi_2(\mathbf{x}_i^\alpha(\omega,t),\mathbf{x}_j^\beta(\omega,t)). \tag{2.9}$$

This has ensemble mean

$$\langle\Phi_2\rangle(t) = \int_{\mathcal{D}}\mathrm{d}\mathbf{x}\int_{\mathcal{D}}\mathrm{d}\mathbf{y}\,\rho_2^{\alpha\beta}(\mathbf{x},\mathbf{y},t)\phi_2(\mathbf{x},\mathbf{y}), \tag{2.10}$$

where formally,

$$\rho_2^{\alpha\beta}(\mathbf{x},\mathbf{y},t) = \int_\Omega p(\mathrm{d}\omega)\sum_{i\in I^\alpha}\sum_{j\in I^\beta}\delta(\mathbf{x}-\mathbf{x}_i^\alpha(\omega,t))\delta(\mathbf{y}-\mathbf{x}_j^\beta(\omega,t)). \tag{2.11}$$

Considering $\mathrm{d}\langle\Phi_2\rangle/\mathrm{d}t$ yields the conservation law

$$\frac{\partial\rho_2^{\alpha\beta}(\mathbf{x},\mathbf{y},t)}{\partial t} + \nabla_{\mathbf{x}}\cdot(\mathbf{v}^{\alpha\beta}(\mathbf{x},\mathbf{y},t)\rho_2^{\alpha\beta}(\mathbf{x},\mathbf{y},t)) + \nabla_{\mathbf{y}}\cdot(\mathbf{v}^{\beta\alpha}(\mathbf{y},\mathbf{x},t)\rho_2^{\beta\alpha}(\mathbf{y},\mathbf{x},t)) = 0 \tag{2.12}$$

(assuming no sources or sinks), where $\mathbf{v}^{\alpha\beta}(\mathbf{x},\mathbf{y},t)$ is defined so that

$$\int_\Omega p(\mathrm{d}\omega)\sum_{i\in I^\alpha}\sum_{j\in I^\beta}\dot{\mathbf{x}}_i^\alpha(\omega,t)\psi_2(\mathbf{x}_i^\alpha(\omega,t)),\mathbf{x}_j^\beta(\omega,t)) =: \int_{\mathcal{D}}\mathrm{d}\mathbf{x}\int_{\mathcal{D}}\mathrm{d}\mathbf{y}\,\rho_2^{\alpha\beta}(\mathbf{x},\mathbf{y},t)\mathbf{v}^{\alpha\beta}(\mathbf{x},\mathbf{y},t)\psi_2(\mathbf{x},\mathbf{y}) \tag{2.13}$$

for any test function $\psi_2(\mathbf{x},\mathbf{y})$. Note that $\rho_2^{\alpha\beta}(\mathbf{x},\mathbf{y},t) = \rho_2^{\beta\alpha}(\mathbf{y},\mathbf{x},t)$. Note also that $\mathbf{v}^\alpha(\mathbf{x},t)$ represents the ensemble mean of the velocity of an α-dislocation at $\mathbf{x}$ at time t, *conditional* upon there being such a dislocation at $\mathbf{x}$ at that time. Similarly, $\mathbf{v}^{\alpha\beta}(\mathbf{x},\mathbf{y},t)$ is the ensemble mean of the velocity of an α-dislocation at $\mathbf{x}$, *conditional* on there being an α-dislocation at $\mathbf{x}$ *and* a β-dislocation at $\mathbf{y}$ at time t.

The continuity Eq. (2.8) of course is well-known; so, in principle, is (2.12), but the velocity terms have been defined perhaps more carefully than is always the case, through the systematic employment of test functions. They will also play a role in the section to follow.

3. The stress due to an array of dislocations

Eqs. (2.8) and (2.12) cannot be solved as they stand, because they contain the velocity terms $\mathbf{v}^\alpha$ or $\mathbf{v}^{\alpha\beta}$. What is needed is a relation between dislocation velocity and stress. The simplest possibility is to invoke the linear kinetic law

$$v = k\tau, \tag{3.1}$$

where v denotes the speed of motion of the dislocation in its glide plane, τ denotes the corresponding resolved shear stress and k is the rate constant. Whether or not this is adopted, it is necessary to discuss the stress produced by the dislocation array. For a dislocation of type α the relevant component of stress at $(\mathbf{x}, t)$ may be given as

$$\tau^\alpha(\mathbf{x}, t, \omega) = \sigma^{A,\alpha}(\mathbf{x}, t) + \sum_\beta \sum_{j\in I^\beta} S^{\alpha\beta}(\mathbf{x}, \mathbf{x}_j^\beta(\omega, t)), \tag{3.2}$$

where $\sigma^{A,\alpha}$ denotes the α-resolved externally-applied stress[1] and $S^{\alpha\beta}(\mathbf{x}, \mathbf{y})$ denotes the α-resolved shear stress at $\mathbf{x}$, generated by a dislocation of type β at $\mathbf{y}$. The sum can extend over all points, including $\mathbf{x}$, if $S^{\alpha\beta}(\mathbf{x}, \mathbf{x})$ is taken to be the "image stress" of the dislocation of type β at $\mathbf{y} = \mathbf{x}$, so that, if the body is infinite, this term is zero. The (unconditional) ensemble mean of this stress is

$$\langle\tau^\alpha\rangle(\mathbf{x}, t) = \int_\Omega p(\mathrm{d}\omega)\tau^\alpha(\mathbf{x}, t, \omega) = \sigma^{A,\alpha}(\mathbf{x}, t) + \sum_\beta \int_{\mathcal{D}} S^{\alpha\beta}(\mathbf{x}, \mathbf{y})\rho_1^\beta(\mathbf{y})\mathrm{d}\mathbf{y}. \tag{3.3}$$

In the case of linear kinetics, Eq. (3.1), any conditional average of the velocity $\mathbf{v}^\alpha$ is related linearly to the corresponding conditional average of τ^α; the case of nonlinear kinetics is more complicated unless it is assumed that the conditional average of $\mathbf{v}^\alpha$ is related just to the corresponding conditional average of τ^α. Such conditional averages are now discussed.

First, $\langle\tau^\alpha\rangle^\alpha(\mathbf{x}, t)$ is defined (*c.f.* (2.6)) so that, for any test function $\psi(\mathbf{x})$,

$$\int_{\mathcal{D}} \rho_1^\alpha(\mathbf{x})\langle\tau^\alpha\rangle^\alpha(\mathbf{x}, t)\psi(\mathbf{x})\mathrm{d}\mathbf{x} = \int_\Omega p(\mathrm{d}\omega) \int_{\mathcal{D}} \tau^\alpha(\mathbf{x}_i^\alpha(\omega, t))\psi(\mathbf{x}) \sum_{i\in I^\alpha} \delta(\mathbf{x} - \mathbf{x}_i^\alpha(\omega, t))\mathrm{d}\mathbf{x}. \tag{3.4}$$

Therefore, employing (3.2) and invoking the definitions (2.4) and (2.11),

$$\rho_1^\alpha(\mathbf{x}, t)\langle\tau^\alpha\rangle^\alpha(\mathbf{x}, t) = \rho_1^\alpha(\mathbf{x}, t)\sigma^{A,\alpha}(\mathbf{x}, t) + \sum_\beta \int_{\mathcal{D}} \rho_2^{\alpha\beta}(\mathbf{x}, \mathbf{y}, t)S^{\alpha\beta}(\mathbf{x}, \mathbf{y})\mathrm{d}\mathbf{y}. \tag{3.5}$$

Next, in correspondence with (2.13), define $\langle\tau^\alpha\rangle^{\alpha\beta}(\mathbf{x}, \mathbf{y}, t)$ by the relation

$$\int_{\mathcal{D}} \mathrm{d}\mathbf{x} \int_{\mathcal{D}} \mathrm{d}\mathbf{y}\, \rho_2^{\alpha\beta}(\mathbf{x}, \mathbf{y}, t)\langle\tau^\alpha\rangle^{\alpha\beta}(\mathbf{x}, \mathbf{y}, t)\phi_2(\mathbf{x}, \mathbf{y}) = \int_\Omega p(\mathrm{d}\omega) \sum_{i\in I^\alpha} \sum_{j\in I^\beta} \tau^\alpha(\mathbf{x}_i^\alpha(\omega, t))\phi_2(\mathbf{x}_i^\alpha(\omega, t), \mathbf{x}_j^\beta(\omega, t)). \tag{3.6}$$

It follows that

$$\rho_2^{\alpha\beta}(\mathbf{x}, \mathbf{y}, t)\langle\tau^\alpha\rangle^{\alpha\beta}(\mathbf{x}, \mathbf{y}, t) = \rho_2^{\alpha\beta}(\mathbf{x}, \mathbf{y}, t)\sigma^{A,\alpha}(\mathbf{x}, t) + \sum_\gamma \int_{\mathcal{D}} \rho_3^{\alpha\beta\gamma}(\mathbf{x}, \mathbf{y}, \mathbf{z}, t)S^{\alpha\gamma}(\mathbf{x}, \mathbf{z})\mathrm{d}\mathbf{z}, \tag{3.7}$$

where, formally, the three-point density $\rho_3^{\alpha\beta\gamma}(\mathbf{x}, \mathbf{y}, \mathbf{z}, t)$ is given by

$$\rho_3^{\alpha\beta\gamma}(\mathbf{x}, \mathbf{y}, \mathbf{z}, t) = \int_\Omega p(\mathrm{d}\omega) \sum_{i\in I^\alpha} \sum_{j\in I^\beta} \sum_{k\in I^\gamma} \delta(\mathbf{x} - \mathbf{x}_i^\alpha(\omega, t))\delta(\mathbf{y} - \mathbf{x}_j^\beta(\omega, t))\delta(\mathbf{z} - \mathbf{x}_k^\gamma(\omega, t)). \tag{3.8}$$

[1] Equivalently, $b^\alpha\sigma^{A,\alpha}$ is the contribution from the applied stress to the Peach–Koehler force on a dislocation of type α, whose Burgers vector has magnitude b^α.

4. Approximations

The mean stress $\langle\tau^\alpha\rangle(\mathbf{x},t)$ is given without approximation by (3.3). Approximations for the conditional mean stresses are now considered.

Here and in the sequel, it is assumed that the positions of the dislocations are uncorrelated at separations that are large relative to a "correlation length" l. Thus,

$$\rho_2^{\alpha\beta}(\mathbf{x},\mathbf{y},t) \sim \rho_1^\alpha(\mathbf{x},t)\rho_1^\beta(\mathbf{y},t) \quad \text{when } |\mathbf{x}-\mathbf{y}|/l \gg 1. \tag{4.1}$$

It is necessary to make a remark about what happens when $\mathbf{y}=\mathbf{x}$. If $\alpha=\beta$, it follows from the definition (2.11) of $\rho_2^{\alpha\beta}(\mathbf{x},\mathbf{y},t)$ with $\alpha=\beta$ that the sum of the terms with $i=j$ is $\rho_1^\alpha(\mathbf{x},t)\delta(\mathbf{y}-\mathbf{x})$. It is assumed that two distinct dislocations may not occupy the same position; thus, there is no term of this type if $\beta\neq\alpha$. It is convenient to write

$$\rho_2^{\alpha\beta}(\mathbf{x},\mathbf{y},t) = \rho_1^\alpha(\mathbf{x},t)\delta_{\alpha\beta}\delta(\mathbf{y}-\mathbf{x}) + \rho_2^{\alpha\beta'}(\mathbf{x},\mathbf{y},t) \tag{4.2}$$

and to expand $\rho_2^{\alpha\beta'}(\mathbf{x},\mathbf{y},t)$ so that

$$\rho_2^{\alpha\beta'}(\mathbf{x},\mathbf{y},t) = \rho_1^\alpha(\mathbf{x},t)\rho_1^\beta(\mathbf{y},t)[1+d_2^{\alpha\beta}(\mathbf{x},\mathbf{y},t)]. \tag{4.3}$$

It follows that the conditional mean stress $\langle\tau^\alpha\rangle^\alpha(\mathbf{x},t)$ is expressible in the form

$$\langle\tau^\alpha\rangle^\alpha(\mathbf{x},t) = \langle\tau^\alpha\rangle(\mathbf{x},t) + S^{\alpha\alpha}(\mathbf{x},\mathbf{x}) + \sum_\beta \int_{\mathcal{D}} S^{\alpha\beta}(\mathbf{x},\mathbf{y})\rho_1^\beta(\mathbf{y},t)d_2^{\alpha\beta}(\mathbf{x},\mathbf{y},t)\mathrm{d}\mathbf{y}. \tag{4.4}$$

Thus, the mean stress experienced by a dislocation at position $\mathbf{x}$ is the unconditional mean stress, plus contributions from its "boundary image stress" and from correlation of the positions of neighbouring dislocations. The contribution from this boundary image term appears not to have been highlighted so explicitly in previous work.

4.1. Mean field approximation

In the mean field approximation, correlations are simply ignored: $d_2^{\alpha\beta}(\mathbf{x},\mathbf{y},t)=0$. In this approximation, the velocity $\mathbf{v}^\alpha(\mathbf{x},t)$ is related to the unconditional mean stress $\langle\tau^\alpha\rangle(\mathbf{x},t)$ and the equations of continuity (2.8) become a closed set for the one-point probabilities $\rho_1^\alpha(\mathbf{x},t)$.

4.2. Correction due to correlations

Use of the exact expression (4.4) requires knowledge of the two-point functions $d_2^{\alpha\beta}(\mathbf{x},\mathbf{y},t)$. They must conform to Eqs. (2.12), in which an expression for $\mathbf{v}^{\alpha\beta}(\mathbf{x},\mathbf{y},t)$ is required. This motivates study of $\langle\tau^\alpha\rangle^{\alpha\beta}(\mathbf{x},\mathbf{y},t)$ which, in turn, requires discussion of the three-point functions $\rho_3^{\alpha\beta\gamma}$. These contain contributions from one and two points. First, if $\alpha=\beta=\gamma$,

$$\begin{aligned}\rho_3^{\alpha\alpha\alpha}(\mathbf{x},\mathbf{y},\mathbf{z},t) = \int_\Omega p(\mathrm{d}\omega)\Bigg\{&\sum_i \delta(\mathbf{x}-\mathbf{x}_i^\alpha(\omega,t))\delta(\mathbf{y}-\mathbf{x})\delta(\mathbf{z}-\mathbf{x})\\ &+\sum_i\sum_{j\neq i}\delta(\mathbf{x}-\mathbf{x}_i^\alpha(\omega,t))\delta(\mathbf{y}-\mathbf{x}_j^\alpha(\omega,t))[\delta(\mathbf{z}-\mathbf{x})+\delta(\mathbf{z}-\mathbf{y})]\\ &+\sum_j\sum_{k\neq j}\delta(\mathbf{y}-\mathbf{x}_j^\alpha(\omega,t))\delta(\mathbf{z}-\mathbf{x}_k^\alpha(\omega,t))\delta(\mathbf{x}-\mathbf{y})\\ &+\sum_i\sum_{j\neq i}\sum_{k\neq i,j}\delta(\mathbf{x}-\mathbf{x}_i^\alpha(\omega,t))\delta(\mathbf{y}-\mathbf{x}_j^\alpha(\omega,t))\delta(\mathbf{z}-\mathbf{x}_k^\alpha(\omega,t))\Bigg\}.\end{aligned} \tag{4.5}$$

Thus

$$\begin{aligned}\rho_3^{\alpha\alpha\alpha}(\mathbf{x},\mathbf{y},\mathbf{z},t) = {}&\rho_1^\alpha(\mathbf{x},t)\delta(\mathbf{y}-\mathbf{x})\delta(\mathbf{z}-\mathbf{x}) + \rho_2^{\alpha\alpha'}(\mathbf{x},\mathbf{y},t)[\delta(\mathbf{z}-\mathbf{x})+\delta(\mathbf{z}-\mathbf{y})] + \rho_2^{\alpha\alpha'}(\mathbf{y},\mathbf{z},t)\delta(\mathbf{x}-\mathbf{y})\\ &+\rho_3^{\alpha\alpha\alpha'}(\mathbf{x},\mathbf{y},\mathbf{z},t),\end{aligned} \tag{4.6}$$

where

$$\rho_2^{\alpha\alpha'}(\mathbf{x},\mathbf{y},t)=\int_\Omega p(\mathrm{d}\omega)\sum_i\sum_{j\neq i}\delta(\mathbf{x}-\mathbf{x}_i^\alpha(\omega,t))\delta(\mathbf{y}-\mathbf{x}_j^\alpha(\omega,t))\equiv\rho_1^\alpha(\mathbf{x},t)\rho_1^\alpha(\mathbf{y},t)[1+d_2^{\alpha\alpha}(\mathbf{x},\mathbf{y},t)] \tag{4.7}$$

and

$$\rho_3^{\alpha\alpha\alpha'}(\mathbf{x},\mathbf{y},\mathbf{z},t)=\int_\Omega p(\mathrm{d}\omega)\sum_i\sum_{j\neq i}\sum_{k\neq i,j}\delta(\mathbf{x}-\mathbf{x}_i^\alpha(\omega,t))\delta(\mathbf{y}-\mathbf{x}_j^\alpha(\omega,t))\delta(\mathbf{z}-\mathbf{x}_k^\alpha(\omega,t)). \tag{4.8}$$

It is useful now to expand $\rho_3^{\alpha\alpha\alpha'}$ as follows:

$$\begin{aligned}\rho_3^{\alpha\alpha\alpha'}(\mathbf{x},\mathbf{y},\mathbf{z},t)&=\rho_1^\alpha(\mathbf{x},t)\rho_2^{\alpha\alpha'}(\mathbf{y},\mathbf{z},t)+\rho_1^\alpha(\mathbf{y},t)\rho_2^{\alpha\alpha'}(\mathbf{z},\mathbf{x},t)+\rho_1^\alpha(\mathbf{z},t)\rho_2^{\alpha\alpha'}(\mathbf{x},\mathbf{y},t)\\&\quad-2\rho_1^\alpha(\mathbf{x},t)\rho_1^\alpha(\mathbf{y},t)\rho_1^\alpha(\mathbf{z},t)+\rho_1^\alpha(\mathbf{x},t)\rho_1^\alpha(\mathbf{y},t)\rho_1^\alpha(\mathbf{z},t)d_3^{\alpha\alpha\alpha}(\mathbf{x},\mathbf{y},\mathbf{z},t).\end{aligned} \tag{4.9}$$

The complete expression for $\rho_3^{\alpha\alpha\alpha}$ follows from (4.6) and (4.9). If $\gamma=\alpha$ or $\gamma=\beta$ and $\alpha\neq\beta$, similar expansions are applicable but they have less terms. The complete expression, for all α,β and γ, is

$$\begin{aligned}\rho_3^{\alpha\beta\gamma}(\mathbf{x},\mathbf{y},\mathbf{z},t)&=\rho_1^\alpha(\mathbf{x},t)\delta_{\beta\alpha}\delta_{\gamma\alpha}\delta(\mathbf{y}-\mathbf{x})\delta(\mathbf{z}-\mathbf{x})+[\rho_2^{\alpha\beta'}(\mathbf{x},\mathbf{y},t)\delta_{\gamma\alpha}\delta(\mathbf{z}-\mathbf{x})+\rho_2^{\alpha\beta'}(\mathbf{x},\mathbf{y},t)\rho_1^\gamma(\mathbf{z},t)]\\&\quad+[\rho_2^{\beta\gamma'}(\mathbf{y},\mathbf{z},t)\delta_{\alpha\beta}\delta(\mathbf{x}-\mathbf{y})+\rho_2^{\beta\gamma'}(\mathbf{y},\mathbf{z},t)\rho_1^\alpha(\mathbf{x},t)]+[\rho_2^{\alpha\beta'}(\mathbf{x},\mathbf{y},t)\delta_{\beta\gamma}\delta(\mathbf{y}-\mathbf{z})\\&\quad+\rho_2^{\gamma\alpha'}(\mathbf{z},\mathbf{x},t)\rho_1^\beta(\mathbf{y})]-2\rho_1^\alpha(\mathbf{x},t)\rho_1^\beta(\mathbf{y},t)\rho_1^\gamma(\mathbf{z},t)\\&\quad+\rho_1^\alpha(\mathbf{x},t)\rho_1^\beta(\mathbf{y},t)\rho_1^\gamma(\mathbf{z},t)d_3^{\alpha\beta\gamma}(\mathbf{x},\mathbf{y},\mathbf{z},t).\end{aligned} \tag{4.10}$$

Evidently, $d_3^{\alpha\beta\gamma}$ tends to zero whenever two of $\mathbf{x}$, $\mathbf{y}$, $\mathbf{z}$ are separated by a large amount in comparison with the correlation length.

The relation (3.7) for $\langle\tau^\alpha\rangle^{\alpha\beta}$ can now be expanded, when $\mathbf{y}\neq\mathbf{x}$, to the form

$$\begin{aligned}\rho_2^{\alpha\beta}(\mathbf{x},\mathbf{y},t)\langle\tau^\alpha\rangle^{\alpha\beta}(\mathbf{x},\mathbf{y},t)&=\rho_2^{\alpha\beta}(\mathbf{x},\mathbf{y},t)[\langle\tau^\alpha\rangle(\mathbf{x},t)+S^{\alpha\alpha}(\mathbf{x},\mathbf{x})+S^{\alpha\beta}(\mathbf{x},\mathbf{y})]+\rho_1^\alpha(\mathbf{x},t)\rho_1^\beta(\mathbf{y},t)\\&\quad\times\sum_\gamma\int_{\mathcal{D}}\rho_1^\gamma(\mathbf{z},t)\left[d_2^{\gamma\alpha}(\mathbf{z},\mathbf{x},t)+d_2^{\beta\gamma}(\mathbf{y},\mathbf{z},t)+d_3^{\alpha\beta\gamma}(\mathbf{x},\mathbf{y},\mathbf{z},t)\right]S^{\alpha\gamma}(\mathbf{x},\mathbf{z})\mathrm{d}\mathbf{z}.\end{aligned} \tag{4.11}$$

An approximate relation, which involves only one- and two-point functions and thus closes the system of equations, is obtained by simply assuming that

$$d_3^{\alpha\beta\gamma}(\mathbf{x},\mathbf{y},\mathbf{z},t)=0. \tag{4.12}$$

This approximation is adopted henceforth.

5. Asymptotic solution for the two-point functions

Regardless of the detail of the kinetic law, it is reasonable to suppose that the force on every dislocation remains finite, and therefore the conditionally-averaged stress component $\langle\tau^\alpha\rangle^{\alpha\beta}(\mathbf{x},\mathbf{y},t)$ must be finite. Since the kernel functions $S^{\alpha\gamma}(\mathbf{x},\mathbf{z})$ become unbounded as $\mathbf{z}$ approaches $\mathbf{x}$, a minimal requirement is that the terms that could be singular in (4.11) must ultimately cancel. Thus, asymptotically, when $\mathbf{x}$ and $\mathbf{y}$ are close and not adjacent to a boundary,

$$(1+d_2^{\alpha\beta}(\mathbf{x},\mathbf{y},t))S^{\alpha\beta}(\mathbf{x}-\mathbf{y})+\sum_\gamma\int\rho_1^\gamma(\mathbf{z})d_2^{\beta\gamma}(\mathbf{y},\mathbf{z})S^{\alpha\gamma}(\mathbf{x}-\mathbf{z})\mathrm{d}\mathbf{z}=0. \tag{5.1}$$

Here $S^{\alpha\gamma}$ has been given as a function of $(\mathbf{x}-\mathbf{z})$ because its asymptotic infinite-body form is implied; likewise, the integral is extended over all space. With just one further approximation, that the unconditional probabilities ρ_1^γ vary slowly with $\mathbf{z}$ on the scale of the correlation length, $\rho_1^\gamma(\mathbf{z})$ can be replaced by $\rho_1^\gamma(\mathbf{x})$. It then becomes consistent to take the two-point functions $d_2^{\beta\gamma}$ to depend on $(\mathbf{y},\mathbf{z})$ only in the combination $(\mathbf{y}-\mathbf{z})$. Eqs. (5.1) then become

$$(1+d_2^{\alpha\beta}(\mathbf{x}-\mathbf{y},t))S^{\alpha\beta}(\mathbf{x}-\mathbf{y})+\sum_\gamma\rho_1^\gamma(\mathbf{x},t)\int d_2^{\beta\gamma}(\mathbf{y}-\mathbf{z},t)S^{\alpha\gamma}(\mathbf{x}-\mathbf{z})\mathrm{d}\mathbf{z}=0. \tag{5.2}$$

6. A single population of screw dislocations

Consider, as a first example, an array of screw dislocations, assumed to be able only to glide in the direction parallel to Ox_1. Since there is only a single population of dislocations, there is only one function d_2. Furthermore, since time enters only through $\rho_1(\mathbf{x},t)$, dependence on time is suppressed. Finally, without loss, $\mathbf{x}$ is taken equal to zero. Eqs. (5.2) thus become

$$(1+d_2(-\mathbf{y}))S(-\mathbf{y})+\rho_1\int d_2(\mathbf{y}-\mathbf{z})S(-\mathbf{z})\mathrm{d}\mathbf{z}=0. \tag{6.1}$$

The relevant stress component, now called simply S, is σ_{23} if the dislocation has Burgers vector $(0,0,b)$ with $b>0$, or $-\sigma_{23}$ if the dislocation has Burgers vector $(0,0,-b)$. Thus, for a positive screw dislocation at $\mathbf{z}$, the stress component σ_{23} at $\mathbf{x}=0$ is

$$S(-\mathbf{z})=-B\frac{z_1}{z_1^2+z_2^2} \tag{6.2}$$

where $B=\mu b/(2\pi)$, with μ the shear modulus of the medium. To evaluate the integral it is convenient to use complex variables introducing $\xi_0=y_1+\mathrm{i}y_2=|\mathbf{y}|\mathrm{e}^{\mathrm{i}\phi}$ and $\xi=(y_1-z_1)+\mathrm{i}(y_2-z_2)=|\xi|\mathrm{e}^{\mathrm{i}\theta}$, such that the shear stress at the origin due to a dislocation at $\mathbf{z}$ is equal to

$$S(-\mathbf{z})=\mathrm{Re}\frac{1}{\xi_0-\xi}, \tag{6.3}$$

where the constant $-B$ is omitted because in any case it cancels through the equation. The analysis to follow will demonstrate the consistency of taking the function $d_2(\mathbf{y}-\mathbf{z})$ to depend only on the distance $r=|\mathbf{y}-\mathbf{z}|$.

The integral in (6.1) can be split into two parts according to the integration regions.

$$\int S(-\mathbf{z})d_2(r)\mathrm{d}\mathbf{z}=\mathrm{Re}\int_{r<|\xi_0|}\frac{1}{\xi_0-\xi}d_2(r)\mathrm{d}\xi+\mathrm{Re}\int_{r>|\xi_0|}\frac{1}{\xi_0-\xi}d_2(r)\mathrm{d}\xi. \tag{6.4}$$

For $r>|\xi_0|$ we get

$$\begin{aligned}\mathrm{Re}\int_{r>|\xi_0|}\frac{1}{\xi_0-\xi}d_2(r)\mathrm{d}\mathbf{z}&=-\mathrm{Re}\int_{|\xi_0|}^{\infty}\int_0^{2\pi}\frac{1}{\xi}\frac{1}{1-\xi_0/\xi}d_2(r)r\,\mathrm{d}r\,\mathrm{d}\theta\\&=-\mathrm{Re}\int_{|\xi_0|}^{\infty}\int_0^{2\pi}\sum_{k=0}^{\infty}\frac{1}{\xi}\left(\frac{\xi_0}{\xi}\right)^k d_2(r)r\,\mathrm{d}r\,\mathrm{d}\theta\\&=-\mathrm{Re}\int_{|\xi_0|}^{\infty}\int_0^{2\pi}\sum_{k=0}^{\infty}\frac{\mathrm{e}^{-\mathrm{i}\theta}}{r}\left(\frac{|\xi_0|}{r}\right)^k\mathrm{e}^{\mathrm{i}k\phi}\mathrm{e}^{-\mathrm{i}k\theta}d_2(r)r\,\mathrm{d}r\,\mathrm{d}\theta=0.\end{aligned} \tag{6.5}$$

For $r<|\xi_0|$,

$$\begin{aligned}\mathrm{Re}\int_{r<|\xi_0|}\frac{1}{\xi_0-\xi}d_2(r)\mathrm{d}\mathbf{z}&=\mathrm{Re}\int_0^{|\xi_0|}\int_0^{2\pi}\frac{1}{\xi_0}\frac{1}{1-\xi/\xi_0}d_2(r)r\,\mathrm{d}r\,\mathrm{d}\theta\\&=\mathrm{Re}\int_0^{|\xi_0|}\int_0^{2\pi}\sum_{k=0}^{\infty}\frac{1}{\xi_0}\left(\frac{\xi}{\xi_0}\right)^k d_2(r)r\,\mathrm{d}r\,\mathrm{d}\theta\\&=\mathrm{Re}\int_0^{|\xi_0|}\int_0^{2\pi}\sum_{k=0}^{\infty}\frac{\mathrm{e}^{-\mathrm{i}\phi}}{|\xi_0|}\left(\frac{r}{|\xi_0|}\right)^k\mathrm{e}^{-\mathrm{i}k\phi}\mathrm{e}^{\mathrm{i}k\theta}d_2(r)r\,\mathrm{d}r\,\mathrm{d}\theta\\&=2\pi\mathrm{Re}\left[\frac{\mathrm{e}^{-\mathrm{i}\phi}}{|\mathbf{y}|}\right]\int_0^{|\mathbf{y}|}d_2(r)r\,\mathrm{d}r=2\pi\frac{\cos(\phi)}{|\mathbf{y}|}\int_0^{|\mathbf{y}|}d_2(r)r\,\mathrm{d}r\\&=2\pi S(-\mathbf{y})\int_0^{|\mathbf{y}|}d_2(r)r\,\mathrm{d}r.\end{aligned} \tag{6.6}$$

Thus, the factor $S(-\mathbf{y})$ cancels through Eq. (6.1), leaving

$$1 + d_2(|\mathbf{y}|) + 2\pi\rho_1 \int_0^{|\mathbf{y}|} d_2(r) r \, \mathrm{d}r = 0. \tag{6.7}$$

Differentiating with respect to $|\mathbf{y}|$ gives a simple first order linear differential equation, with solution

$$d_2(|\mathbf{y}|) = -\mathrm{e}^{-\pi\rho_1|\mathbf{y}|^2}, \tag{6.8}$$

the constant having been chosen so that (6.8) is satisfied. Finally, the two point density function can be written in the form

$$\rho_2'(\mathbf{x},\mathbf{y}) = \rho_1^2(1 - \mathrm{e}^{-\pi\rho_1|\mathbf{x}-\mathbf{y}|^2}). \tag{6.9}$$

7. Screw dislocations of opposite signs

Consider now a system of positive and negative screw dislocations, able to glide in the direction parallel to Ox_1. There are thus two dislocation types, $\alpha = +$ and $\alpha = -$, and if the definition (6.2) is retained for S, then $S^{++} = S^{--} = -S^{+-} = -S^{-+} = S$. It will emerge below that Eqs. (5.2) have no solution in this case, so that some additional physical considerations will be required. However, we first record the equations and then perform some elementary analysis. In an abbreviated notation in which arguments are left implicit, the equations are:

$$\begin{aligned} &(1 + d_2^{++})S + \int (\rho_1^+ d_2^{++} - \rho_1^- d_2^{+-}) S \, \mathrm{d}\mathbf{z} = 0, \qquad -(1 + d_2^{+-})S + \int (\rho_1^+ d_2^{-+} - \rho_1^- d_2^{--}) S \, \mathrm{d}\mathbf{z} = 0, \\ &-(1 + d_2^{-+})S - \int (\rho_1^+ d_2^{++} - \rho_1^- d_2^{+-}) S \, \mathrm{d}\mathbf{z} = 0, \qquad (1 + d_2^{--})S - \int (\rho_1^+ d_2^{-+} - \rho_1^- d_2^{--}) S \mathrm{d}\mathbf{z} = 0. \end{aligned} \tag{7.1}$$

Adding the first and third, and then the second and fourth, of these equations gives

$$d_2^{++} = d_2^{-+}, \quad d_2^{+-} = d_2^{--}. \tag{7.2}$$

Substituting for d_2^{+-} and d_2^{-+} then gives the two equations

$$(1 + d_2^{++})S + \int (\rho_1^+ d_2^{++} - \rho_1^- d_2^{--}) S \, \mathrm{d}\mathbf{z} = 0, \quad (1 + d_2^{--})S - \int (\rho_1^+ d_2^{++} - \rho_1^- d_2^{--}) S \, \mathrm{d}\mathbf{z} = 0. \tag{7.3}$$

Hence,

$$2 + d_2^{++} + d_2^{--} = 0, \tag{7.4}$$

a contradiction, since by hypothesis $d_2^{\alpha\beta}(\mathbf{y} - \mathbf{z})$ decays to zero when $\mathbf{y}$ and $\mathbf{z}$ are widely separated. Note, furthermore, that since this conclusion was reached without invoking the exact form of the kernel S, it would apply equally to arrays of edge dislocations.

A possible resolution is as follows: suppose, to be definite, that $\rho_1^+ > \rho_1^-$. A possibility, not allowed for above, is that all of the negative dislocations could attach themselves to positive dislocations. In the absence of further hypotheses, the dislocation pairs would cancel each other and would, in effect, mutually annihilate, to leave a density $\rho_1^+ - \rho_1^-$ of positive dislocations. In practice, they would more probably form dipoles which would interact only weakly with one another and with the surplus positive dislocations, so that their exact distribution would be indeterminate. In any case, what would be needed is some further injection of physics. It is perhaps worth noting in this context that discrete dislocation simulations have built into them some assumption about close interactions: Van der Giessen et al. (2001) for instance simply assume mutual annihilation if dislocations of opposite sign come within a certain distance of each other. With the assumption of mutual annihilation (or at least disregard) of dislocation pairs, the problem is reduced to the one solved in the preceding section, now with the density ρ_1 taken as the net density $\rho_1^+ - \rho_1^-$ which, incidentally, is the density of "geometrically-necessary dislocations". The solution arrived at in this way is a kind of "limiting case", which might be expected to approximate the results of simulations. It carries no direct implication for simulation results such as those Bakó and Groma (1999), in which dislocations of opposite sign did not annihilate. Dislocation annihilation could be prevented, in the present framework, by modifying the kernel functions

S^{+-} and S^{-+} so that dislocations of opposite signs repelled each other at very close separations. Such a modification would imply that $S^{++} \neq -S^{+-}$ for instance, and would remove at least the "contradiction" developed above. We have made no attempt in this work to pursue further this kind of alternative.

8. Simulations

In order to illustrate the predicted behaviour of the dislocations a small discrete dislocation simulation is performed. In the presented example 128 positive and 64 negative screw dislocations are distributed randomly over a periodic cell $-1/2 \leqslant x_1, x_2, \leqslant 1/2$. The dislocation slip planes are parallel to the Ox_1 axis. The dislocations allocated initially at random are allowed to adjust themselves during the simulation, which is implemented by numerically solving the system of linear motion Eq. (3.1).

In discrete dislocation simulations it is common to use finite element analysis to compute the boundary image stress. In the case of periodic array of dislocations it can be done analytically by direct summation

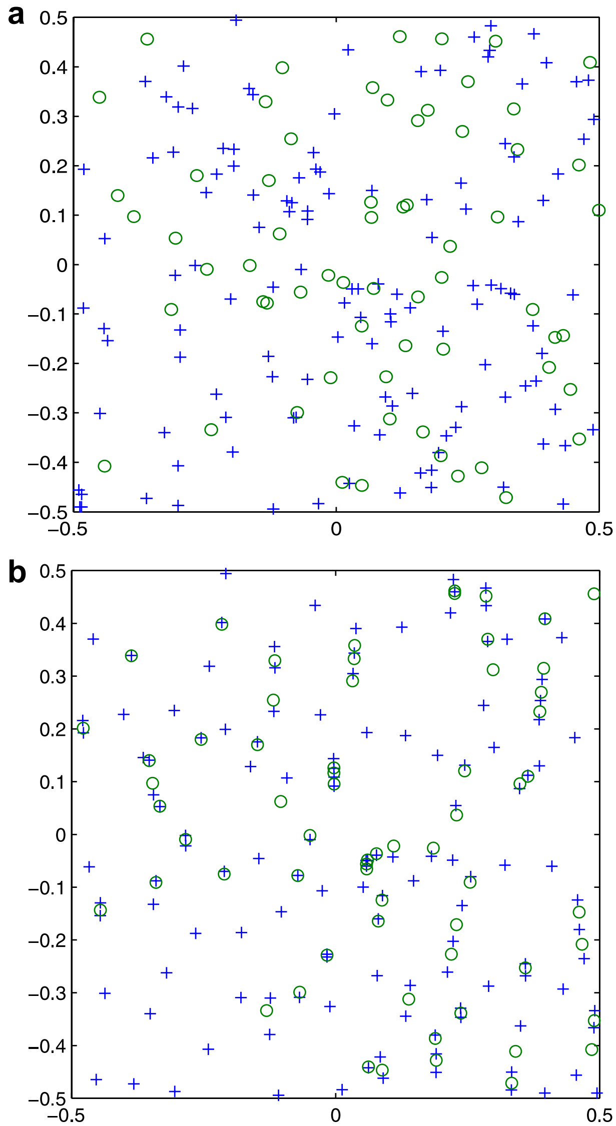

Fig. 1. Initial (a) and relaxed (b) dislocation distributions. The crosses are used to indicate the locations of positive dislocations, and circles indicate negative dislocations.

of the dislocation replica contributions. For example, the shear stress on a positive dislocation at $\mathbf{x}$ due to a positive dislocation at the origin and its replicas is given by

$$S(\mathbf{x}) = B\sum_{k=-\infty}^{\infty}\sum_{m=-\infty}^{\infty}\frac{x_1+k}{(x_1+k)^2+(x_2+m)^2}. \tag{8.1}$$

The correct summation should provide periodic stress field and the right type of singularity at the origin. It is achieved by the following transformation

$$\begin{aligned} S(\mathbf{x}) &= B\sum_{k=-\infty}^{\infty}\sum_{m=-\infty}^{\infty}\frac{x_1+k}{(x_1+k)^2+(x_2+m)^2} \\ &= B\frac{1}{2}\sum_{k=-\infty}^{\infty}\sum_{m=-\infty}^{\infty}\left[\frac{1}{x_1+k+\mathrm{i}(x_2+m)}+\frac{1}{x_1+k-\mathrm{i}(x_2+m)}\right] \\ &= B\frac{\pi}{2}\sum_{m=-\infty}^{\infty}[\cot(\pi(x_1+\mathrm{i}(x_2+m)))+\cot(\pi(x_1-\mathrm{i}(x_2+m)))] \\ &= B\frac{\pi}{2}\sum_{m=-\infty}^{\infty}\frac{\sin(2\pi x_1)}{\cosh^2(\pi(x_2+m))-\cos^2(\pi x_1)}. \end{aligned} \tag{8.2}$$

This series converges very fast: only a few terms with positive and negative m are required to get high accuracy.

The initial and resultant relaxed distributions are shown in Fig. 1. One can observe that the negative dislocations make an attempt to approach the positive ones as close as possible. Due to initially random distribution of the dislocations, they do not necessarily move on the same slip planes. Thus, since no annihilation mechanism is assumed here, attraction of the dislocations of opposite signs results in formation of "dipoles". The interaction of dipoles leads to formation of column-like structures, which minimizes the force a dislocation applies on the dipole neighbour. Similar behaviour was observed by Bakó and Groma (1999) in their discrete dislocation simulations performed for a random array of edge dislocations.

9. Implications for plasticity

Attempts to relate the phenomenon of plastic deformation and the associated continuum theory of plasticity to dislocation dynamics have been made for the last half-century. Early papers include those of Mura (1965, 1967), Berdichevskii and Sedov (1967) and more recent ones include that of Groma (1997) and subsequent contributions mentioned below. The early work of Groma (1997) was explicitly based on equations of motion for dislocations, employing the linear kinetic law (3.1). A hierarchy of equations was generated, and the hierarchy closed by making the "mean field" approximation, in which correlations are ignored. Although developed less formally, the work of Mura (1965, 1967), and others, implicitly makes the same approximation. Groma et al. (2003) allowed for correlations and obtained thereby equations that contained a length scale, associated with the mean spacing of dislocations. A drawback of the approach of Groma (1997) and Groma et al. (2003) is that their resulting continuum description would inevitably reflect the underlying "linear viscosity" of the assumed linear kinetic law. They were able, however, to identify departures from the mean field approximation, resulting from the admission of the two-point correlation, and estimated the new non-local term from the form of the two-point correlation, as obtained from a set of direct discrete-dislocation simulations.

The philosophy to be adopted here is similar in some respects, except that we circumvent the adoption of any kinetic law (linear or nonlinear) and so make no explicit prediction of a set of equations for continuum plasticity. Instead, we note that the (ensemble) mean stress at any point $\mathbf{x}$ is given *exactly* by (3.3), and remark that, in conventional continuum plasticity, the flow law relates the plastic strain-rate at any instant to this mean stress. Now, as anticipated in Section 5, we note (for linear kinetics) or postulate (for nonlinear kinetics) that mean dislocation velocity depends not on the unconditionally-averaged stress, but on the stress averaged conditionally on the presence of a dislocation at the point of interest. The difference between unconditionally- and conditionally-averaged stress is given, *without approximation*, by (4.4). It is this difference that provides departures from conventional continuum plasticity, much more generally than in the case of linear kinetics discussed by Groma et al. (2003). It is perhaps worth noting that the "image stress" term in (4.4) provides a departure from conventional plasticity, resulting in a "size effect", even if the two-point correlation is disregarded. Here, however, our concern is for behaviour "in the bulk", so that the infinite-body form for the kernel S is adopted. Eq. (4.11) gives $\langle\tau^\alpha\rangle^{\alpha\beta}$ exactly, and the argument given in Section 5 that it must contain no singularity as $\mathbf{y}$ approaches $\mathbf{x}$ has to apply. Eq. (5.1) reflect this requirement, having made the closure approximation of neglecting the three-point term $d_3^{\alpha\beta\gamma}$. Zaiser et al. (2001) reach a similar conclusion, based on their study of linear kinetics, but they choose a different approximation to close the system, due to Kirkwood (1938):

$$\rho_3^{\alpha\beta\gamma'}(\mathbf{x},\mathbf{y},\mathbf{z}) = \frac{\rho_2^{\alpha\beta'}(\mathbf{x},\mathbf{y})\rho_2^{\beta\gamma'}(\mathbf{y},\mathbf{z})\rho_2^{\gamma\alpha'}(\mathbf{z},\mathbf{x})}{\rho_1^\alpha(\mathbf{x})\rho_1^\beta(\mathbf{y})\rho_1^\gamma(\mathbf{z})}. \tag{9.1}$$

They discuss the properties of the solution of their equation but do not attempt to solve it, relying instead on direct simulation. Groma et al. (2003) and also Zaiser and Aifantis (2006) make use of the same simulation results.

Now consider the case of antiplane shear of a medium, containing a single set of slip planes parallel to the (x_1, x_3)-plane in which only screw dislocations are activated. In general, decomposing the rate of distortion $\partial\dot{u}_i/\partial x_j$ into elastic and plastic parts thus:

$$\partial\dot{u}_i/\partial x_j = \dot{\beta}_{ij}^e + \dot{\beta}_{ij}^p, \tag{9.2}$$

it follows in the present case that

$$\dot{\beta}_{32}^p = \rho_1^+ v^+ + \rho_1^- v^- = (\rho_1^+ - \rho_1^-)v^+, \tag{9.3}$$

with all other components of $\dot{\beta}_{ij}^p$ equal to zero. A kinetic relation for v^+ thus generates a continuum flow law. Note that $(\rho_1^+ - \rho_1^-)$ is the density of "geometrically-necessary" dislocations, and

$$b(\rho_1^+ - \rho_1^-) = -\partial\beta_{32}^p/\partial x_1. \tag{9.4}$$

Note that it has been assumed that, as defined, $\rho_1 > 0$.

Now employing the solution given in Section 7, with $\mathbf{x}$ taken to define the origin of coordinates, the relation (4.4) gives

$$\langle\tau^+\rangle^+(0) = \langle\tau^+\rangle(0) + \frac{\mu b}{2\pi}\int \frac{y_1}{y_1^2 + y_2^2}\rho_1(\mathbf{y})e^{-\pi\rho_1(0)|\mathbf{y}|^2}\,d\mathbf{y}, \tag{9.5}$$

where here $\rho_1 = \rho_1^+ - \rho_1^-$. To leading order, assuming that ρ_1 varies slowly on the length scale $[\pi\rho_1(0)]^{-1/2}$, so that $\rho_1(\mathbf{y}) \sim \rho_1(0) + \mathbf{y}\cdot\nabla\rho_1(0)$, this relation is, asymptotically,

$$\begin{aligned}\langle\tau^+\rangle^+(0) &\sim \langle\tau^+\rangle(0) + \frac{\mu b}{2\pi}\frac{\partial\rho_1(0)}{\partial x_1}\int_0^\infty\int_0^{2\pi}\cos^2\theta e^{-\pi\rho_1 r^2} r\,dr\,d\theta = \langle\tau^+\rangle(0) + \frac{\mu b}{4\pi\rho_1(0)}\frac{\partial\rho_1(0)}{\partial x_1}\\ &= \langle\tau^+\rangle(0) - \frac{\mu}{4\pi\rho_1(0)}\frac{\partial^2\beta_{32}^p}{\partial x_1^2}.\end{aligned} \tag{9.6}$$

A relation of this form was given by Zaiser and Aifantis (2006), in the context of an array of edge dislocations, except that the constant multiplying the "gradient" term was not calculated precisely. If the present criterion for dislocation motion is $\langle\tau^+\rangle^+ = \tau^{\text{crit}}$, then equation (9.6) implies the continuum yield criterion

$$\langle\tau^+\rangle = \tau^{\text{crit}}\left(1 + l^2\frac{\partial^2\beta_{32}^p}{\partial x_1^2}\right), \tag{9.7}$$

where

$$l^2 = \frac{\mu}{4\pi\rho_1(0)\tau^{\text{crit}}} = \frac{\mu b}{4\pi|\beta_{32,1}^p(0)|\tau^{\text{crit}}}. \tag{9.8}$$

A similar conclusion was reached by Groma et al. (2003); the difference here is that there has been no resort to simulation, nor to any assumption about the form of the kinetic law for the motion of the dislocations. The result (9.7) has the general form proposed phenomenologically by Aifantis (1984); see also Fleck and Hutchinson (2001).

10. Concluding remarks

The main contribution of this work has been a reasonably careful setting up of equations needed to describe the interaction of arrays of dislocations of sufficient geometrical complexity that they are best modelled as random. Their subsequent re-organisation through motion depends on a kinetic law. Here, we have chosen to depart from the common practice of assuming linear kinetics, and have instead pursued the implication of assuming only that the force on any dislocation must remain finite. This permitted the development of equations that must apply to dislocations in close proximity, regardless of the detail of the kinetic law. Of course these equations should apply in any particular case, including linear kinetics. Such equations have been given previously (explicitly for linear kinetics) by Zaiser et al. (2001). The main novelty here is that the system has been closed and a solution of the resulting equation has been found analytically, for a distribution of screw dislocations.

We have tried to follow through the implications of our formulation, without injecting further hypotheses on the way. This led, however to the conclusion that there could be no asymptotic solution at small separations for arrays of dislocations of positive and negative signs. The paradox was resolved by introducing the one further hypothesis that positive and negative dislocations would either form dipole pairs, or else annihilate each other, until one population was eliminated or neutralized. A direct simulation of discrete dislocations provided some support for the hypothesis of dipole formation.

Next, essentially following Groma et al. (2003) (but not assuming any particular kinetic law), some implications were drawn for continuum plasticity theory. It emerged, asymptotically to lowest order in gradient terms, that the yield stress in classical plasticity would be enhanced by a gradient term, in the way proposed by Aifantis (1984) and, later, Fleck and Hutchinson (2001). It should be remarked, too, that the possibility of such dependence was recognised much earlier, by Berdichevskii and Sedov (1967) in a very sophisticated development of plasticity from the theory of continuous distributions of dislocations. It emerges also, from much more recent studies of crystal plasticity, such as Gurtin (2000). Here, anyway, the length scale that enters thereby was calculated explicitly from the pair distribution function of the geometrically-necessary dislocations. The model assumed in the present work, of a population of positive and negative screw dislocations, of course is very special. Furthermore, the asymptotic analysis, although "honest", is subject to all of the limitations assumed in its development. In particular, three-dimensional configurations would allow dislocation entanglement,"statistically-stored" dislocations certainly would remain, and the "geometrically-necessary" dislocations would exist only as resultants and not as identifiable single entities as in the present case. Thus, further "gradient" effects cannot be excluded, but it is interesting that the present completely explicit calculations have demonstrated a clear effect of the geometrically-necessary dislocations.

One final remark is perhaps in order. For application to boundary-value problems, strain-gradient plasticity, as derived in this work, requires the introduction of higher-order boundary conditions, and once these have been selected, scale effects will be predicted. However, even at the level of the "mean field" approximation, the presence of the "image stress" term in (4.4) will provide a scale effect, and only "classical" boundary conditions are required. The question of which effect is the more significant remains to be addressed.

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