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Simulated small-angle scattering patterns for a plastically deformed model composite material

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Abstract. The small-angle scattering patterns predicted by discrete dislocation plasticity versus local and non-local continuum plasticity theory are compared in a model problem. The problem considered is a two-dimensional model composite with elastic reinforcements in a crystalline matrix subject to macroscopic shear. Only single slip is permitted in the matrix material. Emphasis is on the relationship between characteristics of the scattering patterns and the dislocation structures that can develop as a function of the composite morphology. The computed small-angle scattering patterns clearly distinguish between the different dislocation structures that arise for different composite morphologies. Many features of the small-angle scattering patterns are also reproduced by continuum slip plasticity theory, although the local features due to the discreteness of the individual dislocations are not. The non-local hardening description that gives the best fit with the overall stress–strain response is found to also give the best agreement between the non-local continuum and the discrete dislocation scattering patterns.

1. Introduction

Diffraction and small-angle scattering are among the few techniques that allow the experimental determination of stresses, i.e. elastic strains, in samples that have a size between micrometres and fractions of a millimetre. Such experiments are frequently used in materials science to extract information on dislocation structures. A key issue in these experiments is that the interpretation of diffraction profiles or small-angle scattering patterns in terms of dislocation densities requires a model. Various theories are available at the moment, some of which are based on idealized dislocation distributions, for example Wilkens [1] and Groma [2], while others are based on continuum theories of plastic deformation, for example Povirk *et al* [3]. Models for describing plasticity at length scales of interest for diffraction or small-angle scattering are in an early stage of development and have attracted considerable attention in recent years, although for very different reasons.

The main reason for interest in modelling plastic flow on this size scale stems from its size dependence, as demonstrated, for example, by Fleck *et al* [4], Ma and Clarke [5] and Stölken and Evans [6]. Because plastic flow on this size scale is intermediate between scales that are conveniently treated atomistically or by conventional size independent continuum plasticity, new frameworks for solving boundary value problems are being developed. These include discrete dislocation plasticity, for example Cleveringa *et al* [7], and various non-local plasticity theories, for example Fleck and Hutchinson [8], Acharya and Bassani [9],

Arsenlis and Parks [10], Gao *et al* [11] and Gurtin [12]. In the discrete dislocation framework the dislocations are treated as singularities in an elastic medium, so that the stress and deformation fields associated with each dislocation are accounted for. The solution of boundary value problems within the discrete dislocation plasticity framework is computationally very intensive. The non-local continuum plasticity formulations are computationally more convenient, but which, if any, of these theories provides a predictive framework for plastic flow processes on the microscale remains to be determined.

One way of discriminating between the various theories is by comparing predictions of overall behaviour in deformation states such as indentation, torsion or bending with experimental observations. The problem with this is that predictions of overall behaviour are not very discriminating; suitably adjusting parameters can lead to theories with very different physical bases agreeing with a given set of experimental data, see [5]. More discriminating comparisons are based on predictions for the spatial variation of local fields and, at the size scale of micrometres, local field quantities are often most accessible experimentally via diffraction and scattering methods. Therefore, the differences in the predicted scattering patterns for the various plasticity theories provides a quantitative means of differentiating between them.

In this paper we will confine attention to consideration of small-angle scattering patterns in order to analyse the dislocation microstructures in a model composite material. Small-angle scattering from dislocations has been the subject of a number of early theoretical [13–16] and experimental (e.g. [17]) investigations. The theory of small-angle scattering from straight edge dislocations in isotropic linear elastic solids was first developed by Atkinson and Hirsch [13] and was generalized to include non-straight dislocations by Seeger and Kröner [15]. Recently, the theory has been further developed by Shenoy and Phillips [18] using the theory of eigenstrains to include the general case of scattering from dislocations in anisotropic solids. The small-angle theory has been applied by various authors in order to investigate scattering amplitudes from dislocation pile-ups [14], loops [16] and more recently from cell walls [19]. On the experimental side, the availability of powerful synchrotron light sources has led to renewed interest in the analysis of dislocation microstructures using the small-angle scattering method. For example, Levine and coworkers at NIST [20] are currently using the ultra small-angle scattering technique to investigate cell structures in deformed single crystals of metals.

Small-angle scattering patterns predicted by discrete dislocation plasticity and non-local continuum plasticity are compared in a model problem. The problem considered is an idealized two-dimensional composite material with a metal matrix and periodic rectangular elastic reinforcements. The composite is subject to plane strain simple shear with the crystal axes such that the matrix deforms in a single slip. Two composite morphologies analysed by Cleveringa *et al* [7] are considered. In the first, slip cannot propagate across the unit cell without being blocked by the elastic reinforcement. In this case a pattern of geometrically necessary dislocations arises that allows for rotation of the reinforcement. In the other morphology there is a channel of material where slip can propagate unimpeded across the cell. For this composite morphology deformation is focused in a slip band. For the present purposes the role of the composite morphology is to allow for different matrix dislocation structures to arise in a very simple single slip context.

Previously, Cleveringa *et al* [21] considered the mean value and the variance of the (residual) strain distributions for both types, as estimates for the shift and the broadening of diffraction lines. In the present study, the small-angle scattering patterns that emerge from the two types of dislocation structures are calculated. In addition to comparing the small-angle scattering patterns predicted by discrete dislocation plasticity theory and the non-local plasticity theory of Acharya and Bassani [9], we consider the extent to which key features of the dislocation structure can be extracted from the small-angle scattering patterns.

2. Model composite

Cartesian tensor notation is used throughout and a small displacement gradient formulation is employed. A two-dimensional model composite material is analysed that contains elastic rectangular reinforcements in a plastically deforming matrix. The reinforcements are arranged in a doubly periodic hexagonal array as shown in figure 1. Each unit cell is of width $2w$ and height $2c$ ($w/c = \sqrt{3}$) and contains two reinforcements of size $2w_f \times 2c_f$, one being located at the centre of the cell.

Figure 1. Unit cell of a composite material with a doubly-periodic array of elastic reinforcements. All slip planes are taken to be parallel to the applied shear direction (x_1 -direction).

The equilibrium and the strain–displacement relation are expressed by

$$\frac{\partial \sigma_{ij}}{\partial x_j} = 0 \quad (1)$$

and

$$\epsilon_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (2)$$

where u_i is the displacement field, ϵ_{ij} are the strain components and σ_{ij} are the stress components.

The unit cell is subjected to plane strain simple shear in the x_1 -direction, which is prescribed through the boundary conditions

$$u_1(t) = \pm c\Gamma \quad u_2(t) = 0 \quad \text{along } y = \pm c \quad (3)$$

where $\Gamma(t)$ is the applied shear at time t . Periodic boundary conditions are imposed along the lateral sides $x_1 = \pm w$.

2.1. Discrete dislocation plasticity

In the discrete dislocation description of plasticity in the matrix, the dislocations are represented as line defects in a linear elastic continuum (see, e.g., [22, 23]). For the model composite material only edge dislocations on a single slip system are considered, with the slip plane normal being in the x_2 -direction and with the glide direction being in the x_1 -direction, and all dislocations have the same Burgers vector magnitude. The boundary value problem is solved by writing the displacement, strain and stress fields as the superposition of two fields [7, 24]:

$$u_i = \tilde{u}_i + \hat{u}_i \quad \epsilon_{ij} = \tilde{\epsilon}_{ij} + \hat{\epsilon}_{ij} \quad \sigma_{ij} = \tilde{\sigma}_{ij} + \hat{\sigma}_{ij}. \quad (4)$$

The $(\tilde{})$ fields are the superposition of the fields of the individual dislocations in their current configuration, for example,

$$\tilde{u}_i = \sum_k u_i^{(k)} \quad (5)$$

but in an infinite medium of the homogeneous matrix material. The $(\tilde{})$ fields give rise to tractions $\tilde{T}_i$ and displacements $\tilde{u}_i$ on the boundary of the body.

The $(\hat{})$ fields correct for the actual boundary conditions and for the presence of the reinforcements, and satisfy (1) and (2) with

$$\begin{aligned} \hat{\sigma}_{ij} &= \mathcal{L}_{ijkl} \hat{\epsilon}_{kl} && \text{in the matrix } \Omega_m \\ \hat{\sigma}_{ij} &= \mathcal{L}_{ijkl}^* \hat{\epsilon}_{kl} + (\mathcal{L}_{ijkl}^* - \mathcal{L}_{ijkl}) \tilde{\epsilon}_{kl} && \text{in the reinforcement } \Omega_p \end{aligned} \quad (6)$$

where $\mathcal{L}_{ijkl}$ and $\mathcal{L}_{ijkl}^*$ are the matrix and reinforcement elastic moduli, respectively. Assuming elastic isotropy, the matrix moduli are given by

$$\mathcal{L}_{ijkl} = \frac{E}{1+\nu} \left[\frac{1}{2} (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) + \frac{\nu}{1-2\nu} \delta_{ij} \delta_{kl} \right] \quad (7)$$

where E is Young's modulus and ν is Poisson's ratio. The reinforcement moduli are given by an expression of the form (7) with E replaced by E^* and ν by ν^* . For the matrix, we take $E = 70$ GPa and $\nu = 0.33$ giving a shear modulus $\mu = E/2(1+\nu)$ of 26.3 GPa. The corresponding values for the reinforcement are $E = 450$ GPa, $\nu = 0.17$ and $\mu = 192.3$ GPa. These values are representative for silicon carbide particles in an aluminium matrix.

The $(\hat{})$ image fields are smooth and the linear elastic boundary value problem for them can be solved by standard numerical techniques, such as the finite-element method. For the plane strain shear problem here, the boundary conditions for the $(\hat{})$ fields are

$$\hat{u}_i = u_i - \tilde{u}_i \quad \text{along } y = \pm c \quad (8)$$

with u_i prescribed according to (3), together with symmetry conditions along $x = \pm w$.

As described in [7], the deformation history is calculated in an incremental manner. The computations for each time step involve determining the Peach–Koehler forces on the dislocations, determining the change in the dislocation structure and determining the stress and strain state for the updated dislocation arrangement. An initial distribution of dislocation sources and obstacles is specified on each slip plane. Obstacles to dislocation motion are modelled as fixed points on a slip plane. No dislocations are present initially. New dislocations are generated by a two-dimensional Frank–Read sources that generate a dislocation dipole when the magnitude of the Peach–Koehler force at the source exceeds the critical value for a specified period of time. Dislocation motion is assumed to occur only by glide with no cross slip so that dislocations remain on their slip plane. The velocity of each dislocation is taken to be proportional to the Peach–Koehler force on it. Opposite signed dislocations on the same slip plane annihilate when they come within a critical distance. The details of this procedure are not important here but can be found in [7].

2.2. Continuum plasticity

In continuum plasticity theory, the total strain rate is written as the sum of an elastic part, $\dot{\epsilon}_{ij}^e$, and a plastic part, $\dot{\epsilon}_{ij}^p$. Here there is a single slip system so that the plastic strain rate can be written as

$$\dot{\epsilon}_{ij}^p = \frac{\dot{\gamma}}{2}(s_i m_j + s_j m_i) \quad (9)$$

where γ is the slip, s_i specifies the slip direction, m_i is the slip plane normal and $(\cdot)$ denotes differentiation with respect to time. A consequence of (9) is that $\dot{\epsilon}_{ii}^p = 0$. The Schmidt resolved shear stress, given by

$$\tau = s_i \sigma_{ij} m_j \quad (10)$$

is work conjugate to $\dot{\gamma}$ in that $\tau \dot{\gamma} = \sigma_{ij} \dot{\epsilon}_{ij}^p$.

The non-local continuum plasticity formulation adopted in [25] is based on the simple theory proposed by Acharya and Bassani [9] where a particular strain gradient, which is taken to be a measure of elastic (or plastic) incompatibility, enters the flow rule only through the instantaneous hardening rate. For single slip in plane strain, with s_1 in the x_1 -direction, the hardening relation used in [25] is

$$\dot{\gamma} = \dot{\gamma}_0 \left(\frac{\tau}{g} \right) \left(\left| \frac{\tau}{g} \right| \right)^{(1/m)-1} \quad (11)$$

where $\dot{\gamma}_0$ is a reference strain rate and m is the strain rate hardening exponent. The hardness g has an initial value g_0 and is taken to evolve according to

$$\dot{g} = h \left(\gamma, \frac{\partial \gamma}{\partial x_1} \right) \dot{\gamma} \quad (12)$$

together with a power-law hardening relation of the form

$$h \left(\gamma, \frac{\partial \gamma}{\partial x_1} \right) = h_0 \left(\frac{\gamma}{\gamma_0} - 1 \right)^{N-1} \left[1 + \ell^2 \left(\frac{1}{\gamma_0} \frac{\partial \gamma}{\partial x_1} \right)^2 \right]^p \quad (13)$$

where ℓ is the intrinsic length scale, and N , h_0 , γ_0 and p are material parameters. For $\ell = 0$ the local theory is recovered.

The significance of the slip gradient $\partial \gamma / \partial x_1$ in (13) stems from its relation to the net Burgers vector B_i accompanying crystallographic slip, which is given by

$$B_i = \int_{\Omega} \alpha_{ij} v_j d\Omega. \quad (14)$$

Here, Ω is a surface generated by a cut in the crystal, v_i is the outward normal to Ω and α_{ij} is Nye's dislocation density tensor. For single slip in two dimensions, with the slip plane normal in the x_2 -direction, the only non-zero component of α_{ij} is α_{13} , which is given by

$$\alpha_{13} = \frac{\partial \gamma}{\partial x_1}. \quad (15)$$

The relations (9)–(13), together with the elastic relation

$$\epsilon_{ij}^e = \mathcal{L}_{ijkl}^{-1} \sigma_{kl} \quad (16)$$

specify the matrix behaviour. The response of the reinforcement is simply $\sigma_{ij} = \mathcal{L}_{ijkl}^* \epsilon_{kl}$.

With the constitutive response of the matrix and reinforcement specified, this formulation leads to a standard rate boundary value problem that is solved by a finite-element method, as described by Bassani *et al* [25]. The deformation history is then calculated in a linear incremental manner.

3. Synopsis of the scattering analysis

We will now describe the theory of small-angle x-ray or neutron scattering analysis used to study the deformation-induced dislocation microstructures in the model composite material. We will reformulate the small-angle scattering theory [13–16, 18] originally developed for dislocations in infinite homogeneous solids to include the image fields discussed in section 2.

Consider a beam of x-rays or neutrons incident on the composite material. The wave function of the incident waves has the spatial variation $\exp(\mathbf{k} \cdot \mathbf{x})$, where the wavevector is given by $\mathbf{k} = k_1 \mathbf{e}_1 + k_2 \mathbf{e}_2$. All inhomogeneities in the composite material scatter the x-rays in different directions. The wave function of the scattered waves has the spatial variation $\exp(i\mathbf{k}' \cdot \mathbf{x})$, with $\mathbf{k}' = \mathbf{k} + \mathbf{q}$, where $\mathbf{k}' - \mathbf{k} = \mathbf{q} = q_1 \mathbf{e}_1 + q_2 \mathbf{e}_2$, is the scattering vector. The intensity of the scattered waves is conveniently expressed in terms of the scattering amplitude $S(\mathbf{q})$ as [14, 16, 26]

$$I(\mathbf{q}) = |a_e|^2 S(\mathbf{q}) S^*(\mathbf{q})$$

$$S(\mathbf{q}) = \int_{\Omega} \rho(\mathbf{x}) \exp(i\mathbf{q} \cdot \mathbf{x}) d\mathbf{x} \quad (17)$$

where $\rho(\mathbf{x})$ is the local electron density and a_e is a proportionality constant related to the scattering intensity of one electron at the incident intensity of the x-rays or neutrons. The integral is taken over the entire (infinite) region $\Omega = \Omega_m \cup \Omega_p$ occupied by the composite material. It is clear from (17) that $S(\mathbf{q})$ is the Fourier transform of the local electron density. Note that some authors include a factor 2π in the exponential term; here, this is incorporated in $\mathbf{q}$.

In (17) attention is restricted to the small-angle scattering regime in which the condition $|\mathbf{q}|a \ll 1$ (a is a length scale of the order of the lattice parameter of the composite material) is satisfied. We can understand this condition by appealing to figure 2, where we have shown the three vectors $\mathbf{k}$, $\mathbf{k}'$ and $\mathbf{q}$. Since we are concerned with elastic scattering, the condition $|\mathbf{k}| = |\mathbf{k}'|$ is satisfied. It therefore follows that

$$|\mathbf{q}| = 2|\mathbf{k}| \sin(\theta/2) \quad (18)$$

where θ is the scattering angle (see figure 2). In the small-angle scattering regime where $\theta \ll 1$, the condition $|\mathbf{q}|a \ll 1$ is satisfied, since for x-rays or neutrons $|\mathbf{k}|$ is comparable to $1/a$. In this limit, the intensity of the incident beam scattered in the direction $\mathbf{k}'$, $I(\mathbf{q})$, is proportional to the Fourier transform of the auto-correlation function of the local electron density.

Figure 2. The geometry of the incident wavevector $\mathbf{k}$, the final wavevector $\mathbf{k}'$ and the scattering vector $\mathbf{q}$ along with the scattering angle θ .

It is instructive to first consider the small-angle scattering from the composite materials discussed in section 2 in their undeformed states. Let ρ_m and ρ_p be the average electron density in the matrix and the reinforcements respectively. Using (17), we can write

$$S(\mathbf{q}) = \int_{\Omega} \rho_m \exp(i\mathbf{q} \cdot \mathbf{x}) d\mathbf{x} + \int_{\Omega_p} (\rho_p - \rho_m) \exp(i\mathbf{q} \cdot \mathbf{x}) d\mathbf{x} \quad (19)$$

where the first integral is taken over the entire solid, while the second integral is taken over the reinforcements. The first integral vanishes unless $|\mathbf{q}| = 0$. Using the above equation, it is

then clear that materials with large differences between the matrix and reinforcement electron densities scatter the x-rays very strongly. An analysis of these scattered intensities provide information about the sizes and spatial distribution of the reinforcements. Indeed, when the electron densities of the matrix and the reinforcement are significantly different, the effects of the matrix dislocation microstructures are obscured because scattering due to the differences in the electron densities between the matrix and the reinforcement and that due to the dislocations in the matrix cannot be separated. For example, the electron density of SiC is 88% of that of Al and this contributes significantly to the total scattering amplitude.

Since, for our purposes, the reinforcements merely provide a means of obtaining dislocation structures in the matrix, we consider a hypothetical situation where the electron densities in the matrix and the reinforcements are identical. In such a material, with electron density ρ_e in the undeformed configuration, the local electron density in the deformed state, for small strains can be written as $\rho(\mathbf{x}) = \rho_e[1 + u_{i,i}(\mathbf{x})]$. Using this expression in (17), we can write

$$S(\mathbf{q}) = \rho_e \int_{\Omega} u_{i,i}(\mathbf{x}) \exp(i\mathbf{q} \cdot \mathbf{x}) d\mathbf{x} \quad (20)$$

for all scattering vectors with $|\mathbf{q}| \neq 0$, since the integral $\int \exp(i\mathbf{q} \cdot \mathbf{x}) d\mathbf{x}$ vanishes when evaluated over a solid of infinite extent. In what follows we will first describe the procedure that is used to evaluate (20) in the discrete dislocation formulation followed by a discussion of the procedure used in the case of the continuum plasticity formulation.

Because of the periodicity of the reinforcement microstructure, the region Ω naturally breaks up in a $n_1 \times n_2$ array of composite unit cells. As we will show below the total scattering amplitude is determined from the scattering amplitude computed for any one of the composite unit cells, like that shown in figure 1. We choose this cell Ω_0 to be the one centred at the origin of the (x_1, x_2) coordinate system.

In the case of the discrete dislocation model, the scattering amplitude has contributions from the dislocation fields and the image fields. Using the notation introduced in section 2.1, we can write $S(\mathbf{q}) = \tilde{S}(\mathbf{q}) + \hat{S}(\mathbf{q})$, where $\tilde{S}(\mathbf{q})$ [$\hat{S}(\mathbf{q})$] is obtained by replacing $u_{i,i}(\mathbf{x})$ by $\tilde{u}_{i,i}(\mathbf{x})$ [$\hat{u}_{i,i}(\mathbf{x})$] in (20).

In order to compute the dislocation contribution $\tilde{S}(\mathbf{q})$ to the scattering amplitude, first note that each dislocation k at position $\mathbf{R}^{(k)}$ in the central cell has a replica in all other cells; the replica in cell (n_1, n_2) has position ${}^{(n_1, n_2)}\mathbf{R}^{(k)}$ which can be written as

$${}^{(n_1, n_2)}\mathbf{R}^{(k)} = \mathbf{R}^{(k)} + 2wn_1\mathbf{e}_1 + 2cn_2\mathbf{e}_2. \quad (21)$$

The total displacement field $\tilde{u}_i$ to be used in (20) is the sum of all dislocations (cf (5)), and the contribution of any (n_1, n_2) replica is related to that of the original in the central cell $(0,0)$, $u_i^{(k)}(\mathbf{x})$, through

$${}^{(n_1, n_2)}u_i^{(k)}(\mathbf{x}) = u_i^{(k)}[\mathbf{x} - (2wn_1\mathbf{e}_1 + 2cn_2\mathbf{e}_2)]. \quad (22)$$

Making use of this, the scattering amplitude due to all dislocations can be expressed as

$$\tilde{S}(\mathbf{q}) = \tilde{S}_0(\mathbf{q}) \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} \exp[i(2wn_1q_1 + 2cn_2q_2)] \quad (23)$$

where $\tilde{S}_0(\mathbf{q})$ is the contribution of only the dislocations in the central cell,

$$\tilde{S}_0(\mathbf{q}) = \rho_e \int_{\Omega} \sum_k u_{i,i}^{(k)}(\mathbf{x}) \exp(i\mathbf{q} \cdot \mathbf{x}) d\mathbf{x}. \quad (24)$$

Next, we note that the dislocations in the composite cell appear pair-wise. For each dislocation k with Burgers vector $\mathbf{b} = b\mathbf{e}_1$ in the positive x_1 -direction, at position $\mathbf{R}^{(k)+}$,

there is an opposite dislocation with position $\mathbf{R}^{(k)-}$. Now, the displacement field due to any dislocation at $\mathbf{R}^{(k)}$ can be expressed in terms of that for a dislocation at the origin as $u_i^{(k)}(\mathbf{x}) = u_i^{(0)}(\mathbf{x} - \mathbf{R}^{(k)})$. Substituting this into (24) we arrive at

$$\tilde{S}_0(\mathbf{q}) = \tilde{S}^d(\mathbf{q}) \left(\sum_k \exp(i\mathbf{q} \cdot \mathbf{R}^{(k)+}) - \sum_k \exp(i\mathbf{q} \cdot \mathbf{R}^{(k)-}) \right) \quad (25)$$

with $\tilde{S}^d(\mathbf{q})$ being the scattered intensity of a single positive dislocation at the origin,

$$\tilde{S}^d(\mathbf{q}) = \rho_e \int_{\Omega} u_{i,i}^{(0)}(\mathbf{x}) \exp(i\mathbf{q} \cdot \mathbf{x}) d\mathbf{x}. \quad (26)$$

Using the well known linear elastic displacement field for edge dislocations [22, 23], the latter can be computed to be

$$\begin{aligned} \tilde{S}^d(\mathbf{q}) &= -\rho_e \frac{b}{2\pi} \frac{(1-2\nu)}{(1-\nu)} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{x_2}{x_1^2 + x_2^2} \exp[i(q_1 x_1 + q_2 x_2)] dx_1 dx_2 \\ &= -i\rho_e \frac{(1-2\nu)}{(1-\nu)} \frac{bq_2}{q_1^2 + q_2^2}. \end{aligned} \quad (27)$$

We now pause to point out that the scattering amplitude we computed in (25) can indeed provide vital information on the dislocation microstructure, including the sign and spatial distribution of the dislocations. In order to illustrate this we will compute the scattering amplitudes for the six dislocation structures shown in figure 3. All of these structures are assumed to be present in an infinite solid with the elastic properties of the matrix. For case (a), we have two positive edge dislocations located at $(\pm d_0/2, 0)$, while in case (b) there is one positive and one negative dislocation located at $(-d_0/2, 0)$ and $(d_0/2, 0)$ respectively. Using (25) it is easy to show that the scattering amplitudes in the two cases are given by $\tilde{S}^{(a)}(\mathbf{q}) = 2\tilde{S}^d(\mathbf{q}) \cos(q_1 d_0/2)$ and $\tilde{S}^{(b)}(\mathbf{q}) = -2i\tilde{S}^d(\mathbf{q}) \sin(q_1 d_0/2)$, respectively. Now in cases (c) and (d), where the dislocations are symmetrically placed along the y -axis, the scattering amplitudes are given by $\tilde{S}^{(c)}(\mathbf{q}) = 2\tilde{S}^d(\mathbf{q}) \cos(q_2 d_0/2)$ and $\tilde{S}^{(d)}(\mathbf{q}) = -2i\tilde{S}^d(\mathbf{q}) \sin(q_2 d_0/2)$, respectively. This simple example clearly shows that the scattering amplitudes can be used to distinguish both the sign and the spatial distribution of the dislocations. Now, let us consider cases (e) and (f), where positive dislocations are periodically arranged at $(nd_0, 0)$ and $(0, nd_0)$, respectively, $(n = -\infty, \dots, \infty)$. Using a similar argument that led to (23), but now for a singly-periodic arrays of cells with size d_0 , for case (e) we have $\tilde{S}^{(e)}(\mathbf{q}) \propto \sum_{n=-\infty}^{\infty} \tilde{S}^d(\mathbf{q}) \delta_{q_1, nq_0}$, while in case (f) we get $\tilde{S}^{(f)}(\mathbf{q}) \propto \sum_{n=-\infty}^{\infty} \tilde{S}^d(\mathbf{q}) \delta_{q_2, nq_0}$. Here, δ_{q_i, nq_0} indicates that the scattering amplitude vanishes unless $q_i = nq_0$, with $q_0 = 2\pi/d_0$. Note that the $\mathbf{q}$ dependence of the scattering amplitude can be used to distinguish the spatial distribution of the dislocations in the two cases.

The contribution to $S(\mathbf{q})$ from the image fields can be computed by noting that $\hat{u}_i(\mathbf{x})$ inherits the periodicity of the model composite material, i.e.

$$\hat{u}_i(\mathbf{x}) = \hat{u}_i(\mathbf{x} - (2wn_1\mathbf{e}_1 + 2cn_2\mathbf{e}_2)). \quad (28)$$

Making use of this, it is straightforward to show that

$$\hat{S}(\mathbf{q}) = \hat{S}_0(\mathbf{q}) \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} \exp[i(2wn_1q_1 + 2cn_2q_2)] \quad (29)$$

where $\hat{S}_0(\mathbf{q})$ is just the contribution of the displacement fields inside the central cell, as given by

$$\begin{aligned} \hat{S}_0(\mathbf{q}) &= \rho_e \int_{\Omega_0} \hat{u}_{i,i}(\mathbf{x}) \exp(i\mathbf{q} \cdot \mathbf{x}) d\mathbf{x} \\ &= \rho_e \int_{-w}^w \int_{-c}^c \hat{u}_{i,i}(x_1, x_2) \exp[i(q_1 x_1 + q_2 x_2)] dx_1 dx_2. \end{aligned} \quad (30)$$

Figure 3. Simple dislocation configurations in an infinite solid.

The above expression is evaluated from the image displacement fields that are determined using the finite-element method described in section 2. We evaluated this expression by first computing the contribution arising from each of the individual elements and then summing the contributions from all the elements. The contribution arising from each of the elements were evaluated in closed form by using $\hat{u}_{i,i}(x_1, x_2)$ obtained by using a finite-element interpolation of the nodal displacement fields of the element.

The final expression for the scattering amplitude $S(\mathbf{q})$ can now be written in a convenient form, using (23) and (29), as

$$S(\mathbf{q}) = S_0(\mathbf{q}) \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} \exp[i(2wn_1q_1 + 2cn_2q_2)] \quad (31)$$

where

$$S_0(\mathbf{q}) = \hat{S}_0(\mathbf{q}) + \tilde{S}_0(\mathbf{q}). \quad (32)$$

The double sum in the above expression vanishes unless $(q_1, q_2) = (\pi p/w, \pi q/c)$ (p and q being integers), when the phase factor in the sum is unity. At these $\mathbf{q}$ values, $S(\mathbf{q})$ is proportional to $S_0(\mathbf{q})$, the proportionality constant being the total number of composite unit cells.

In the continuum plasticity formulation, the scattering amplitude is computed by once again making use of periodicity in the same way, leading to (29). Thus, we again arrive at

(31), but with $S_0(\mathbf{q})$ evaluated by using $u_{i,i}(\mathbf{x})$ instead of $\hat{u}_{i,i}(\mathbf{x})$ in (30). In this continuum description we can write $u_{i,i} = \epsilon_{ii}^e + \epsilon_{ii}^p$, but since there is no plastic dilation, only the elastic strain contributes to scattering, $u_{i,i} = \epsilon_{ii}^e$. This elastic strain field can be computed at each stage of the deformation process from the current stress field by using (16). It should also be pointed out, while the total displacement fields are compatible, the elastic and the plastic components themselves are not compatible. The computation of the scattering amplitudes from the finite-element results is performed in the same way as that of $\tilde{S}_0(\mathbf{q})$.

Information about the positions of geometrically necessary dislocations, in some average sense, is contained in Nye's dislocation density given in (15). This field, $\alpha_{13}(\mathbf{x})$, can then be used to construct the dilational field due to these dislocations, $u_{ii}^d(\mathbf{x})$, according to

$$u_{ii}^d(\mathbf{x}) = \int_{\Omega} u_{ii}^{d0}(\mathbf{x} - \mathbf{x}') \alpha_{13}(\mathbf{x}') d\mathbf{x}' \quad (33)$$

where $u_{ii}^{d0}(\mathbf{x})$ is the dilational field of a dislocation with unit Burgers vector located at the origin.

Using the fact that $\alpha_{13}(\mathbf{x})$ is periodic with the periodicity of the composite unit cell, we can write a scattering amplitude analogous to (23) as

$$S^d(\mathbf{q}) = S_0^d(\mathbf{q}) \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} \exp[i(2wn_1q_1 + 2cn_2q_2)] \quad (34)$$

where

$$S_0^d(\mathbf{q}) = b^{-1} \tilde{S}^d(\mathbf{q}) \int_{-w}^w \int_{-c}^c \alpha_{13}(x_1, x_2) \exp[i(q_1x_1 + q_2x_2)] dx_1 dx_2 \quad (35)$$

with $\tilde{S}^d(\mathbf{q})$ given by (27). The Fourier transform of $\alpha_{13}(x_1, x_2)$ in (35) can be evaluated using the procedure described to compute (30). Note that (35) can be evaluated using either a local or a non-local plasticity theory. Also note that (35) only contains the contribution of the net Burgers vector; the contribution to the scattering of statistical dislocations (those having an average Burgers vector of zero) is ignored in (35).

4. Results and discussion

4.1. Discrete dislocation simulations

Figure 4 shows dislocation distributions in the initial configuration for two of the reinforcement morphologies considered by Cleveringa *et al* [7]. In both cases, the cell size is given by $c = 1 \mu\text{m}$ and the area fraction of the reinforcing phase is 20% for both reinforcement morphologies. In figure 4(a), for the morphology termed material (i) ($c_f = w_f = 0.416 \mu\text{m}$), there is a vein of unreinforced material. Since the motion of dislocations in a vein is not blocked by the reinforcement, this leads to a progressive concentration of all dislocation activity into one of the veins in the cell at rather small strains. On the other hand, for the reinforcement morphology termed material (iii) ($c_f = 2w_f = 0.591 \mu\text{m}$), shown in figure 4(b), there is no vein of unreinforced matrix. Because of this, the central reinforcement must rotate to accommodate the shear, with a strong piling up of dislocations against the reinforcement sides. These are the geometrically necessary dislocations of Ashby [27].

The meshes in figure 5 show the deformed configurations for materials (i) and (iii). In each case, the displacements are multiplied by a factor of 10. For material (i) the deformation is concentrated in a single band, while for material (iii) the rotation of the central reinforcement is the dominant feature.

Figure 4. Dislocation distributions in material (i) and material (iii) at $\Gamma = 0.58\%$ and $\Gamma = 0.96\%$, respectively.

The dislocation structures in figure 4 give rise to very different dilation fields, $u_{i,i}(x_1, x_2)$, as shown in figure 6. For material (i), the shear band gives rise to a narrow band of volume change that is dilational for $x_1 > 0$ and compressive for $x_1 < 0$. The volume change is very small outside the band. For material (iii) there are alternate bands of positive and negative dilation emanating from the corners of the central reinforcement that are consistent with its clockwise rotation. The computed scattering intensities are shown in figure 7. Since the intensity is proportional to $|S|^2$, as seen in (17), we plot normalized values of $|S|^2$ in figure 7. Also, note that the range of scattering intensities shown spans five orders of magnitude.

There are two length scales associated with the shear band structure in material (i). The larger length scale is the length of the shear band, which is same as the width of the composite unit cell, and the smaller length scale is the spacing between the slip planes. In distinct contrast, there are several length scales in the dislocation structures associated with the dislocation structures observed in material (iii). These are the width and height of the reinforcements, the mean spacing between the geometrically necessary dislocations at the particle matrix interface, the lengths and the widths of the slip band structures seen in figure 5(b) and a spacing that corresponds to an average distance between the randomly distributed dislocations in figure 4(b). One way of understanding the scattering patterns from such structures is to consider certain idealized dislocation structures.

Figure 5. Deformed meshes computed using the discrete dislocation formulation: (a) material (i) at $\Gamma = 0.58\%$ and (b) material (iii) at $\Gamma = 0.96\%$. The displacements are multiplied by a factor of 10.

4.2. Idealized dislocation structures

In order to interpret the scattering amplitudes obtained from the discrete dislocation simulations it is worth studying the scattering intensities from some representative idealized dislocation structures. To this end we will consider scattering intensities from the four structures shown in figure 8. The first structure, figure 8(a), has an arrangement of dislocations in carpets of dipoles that is similar to the dislocation structure that developed in material (i), see figure 4(a), as a consequence of the localized shearing. The other three structures are considered in order to understand the scattering intensities arising from material (iii). These include dislocation arrangements akin to the pile up of geometrically necessary dislocations at the central particle–matrix interface, figure 8(b), a combination of the geometrically necessary dislocations and dipolar carpet structure, figure 8(c), and a combination of the geometrically necessary dislocations and a random arrangement of dislocations whose Burgers vectors add to zero, figure 8(d). In order to bring out the features of scattering by the above idealized structures we will study, in figure 9, the scattering intensities from all of these idealized

Figure 6. Contours of $u_{i,i}$ computed using the discrete dislocation formulation: (a) material (i) at $\Gamma = 0.58\%$ and (b) material (iii) at $\Gamma = 0.96\%$.

structures that are periodically repeated in every composite unit cell, without adding the fields that correct for the actual boundary conditions as described by (8). This simplification also allows us to derive closed form expressions for the scattering intensities for the cases in figures 8(a)–8(c).

First consider the dipolar carpet configuration shown in figure 8(a). Here, there are a total of $4n_{sb}$ dislocations, with equal numbers of positive and negative dislocations. Using the notation shown in figure 8(a), it can be shown that the scattering amplitude of this configuration is given by

$$S^{sb}(\mathbf{q}) = \tilde{S}^d(\mathbf{q}) e^{i(q_1 x_{10} + q_2 x_{20})} \left[\frac{e^{iq_1 n_{sb} \Delta_1} - 1}{e^{iq_1 \Delta_1} - 1} \right] [1 - e^{-iq_2 \Delta_2}] [1 - e^{-iq_1 n_{sb} \Delta_1}]. \quad (36)$$

It is clear from the above equation that the scattering amplitude vanishes at $q_1 = 2\pi n_1 / (n_{sb} \Delta_1)$

Figure 7. Small-angle scattering intensities computed using the discrete dislocation formulation: (a) material (i) at $\Gamma = 0.58\%$ and (b) material (iii) at $\Gamma = 0.96\%$. The components q_1 and q_2 of the scattering vector have units $1 \mu\text{m}^{-1}$.

and at $q_2 = 2\pi n_2/\Delta_2$, where n_1 and n_2 are integers. It is also evident that the spacing between the peaks in the q_2 -direction is $2\pi/\Delta_2$, while in the q_1 -direction, the spacing between the peaks is $2\pi/(n_{sb}\Delta_1)$. Note that in this case $n_{sb}\Delta_1 = w$, the width of the composite unit cell. Let us first consider the spacing between the peaks in the q_1 -direction. It can be seen from figure 9(a) that the peaks in the q_1 -direction are spaced at distances of $2\pi/w = 3.62 \mu\text{m}^{-1}$ with the intensity of the peaks decreasing with increasing q_1 . The strongest peaks are located at $\pm\pi/w$. Unlike the small peak spacings along the q_1 -direction determined by the length of the slip band, the peak spacings in the q_2 -direction, determined by the spacing Δ_2 between the dislocation

Figure 8. Idealized dislocation distributions. (a) A dipolar carpet structure like that found in material (i). (b) An array of geometrically necessary dislocations along the reinforcement-matrix boundary like that found in material (iii). (c) An array of geometrically necessary dislocations and two dipolar carpets of dislocations in between particles. (d) An array of geometrically necessary dislocations along the reinforcement-matrix boundary and a random distribution of dislocations whose Burgers vectors add to zero.

carpets, are very large. In the q_2 -direction, the points $\pm 2\pi/\Delta_2$, where the scattering amplitude first vanishes, lie far outside the region shown in the figure (using $\Delta_2 = 0.025 \mu\text{m}$, we find that these points correspond to $q_2 = \pm 251 \mu\text{m}^{-1}$).

(d)

Figure 8. (Continued)

We now turn to the configuration in figure 8(b). In this case there are a total of $2n_{gn}$ dislocations with equal numbers of positive and negative dislocations on each side of the particle. We now find that the scattering amplitude can be expressed as

$$S^{gn}(\mathbf{q}) = \tilde{S}^d(\mathbf{q}) e^{i(q_1 x_{10} + q_2 x_{20})} \left[\frac{e^{iq_2 n_{gn} \Delta_2} - 1}{e^{iq_2 \Delta_2} - 1} \right] [1 - e^{-iq_1 2w_f}]. \quad (37)$$

Using the fact that $n_{gn} \Delta_2 = 2c_f$, we find that the scattering amplitude vanishes at $q_1 = 2\pi n_1 / (2w_f)$ and $q_2 = 2\pi n_2 / (2c_f)$, where n_1 and n_2 are integers, with peak spacings of π/w_f and π/c_f in the q_1 and q_2 directions, respectively. Using the numerical values $w_f = 0.294 \mu\text{m}$ and $c_f = 0.591 \mu\text{m}$, we find the peak spacings in the q_1 -direction to be $10.79 \mu\text{m}^{-1}$ and the spacing in the q_2 -direction to be $5.31 \mu\text{m}^{-1}$. This kind of peak structure is observed in the scattering intensities shown in figure 9(b).

In the case of figure 8(c) there are both geometrically necessary dislocations as well as dislocations in a carpet structure, but with a width Δ_2 that is significantly larger than in figure 8(a). In this case, the scattering amplitude can be expressed as a sum of the scattering amplitudes according to the expressions (36) and (37). The combined effect of these two structures makes it difficult to derive expressions for peak spacings in closed form. However, the new features arising from the slip band can be seen in figure 9(c). One such new feature is the appearance of peaks in the q_2 -direction at $q_1 = \pm\pi/w$. These peaks are spaced at intervals of length $2\pi/\Delta_2 = 19.04 \mu\text{m}^{-1}$, where $\Delta_2 = 0.33 \mu\text{m}$ is the spacing between dislocation carpets as shown in figure 9(c). Unlike the carpet spacing in material (i) or in figure 8(a), here the slip band spacing is much larger so that several of these peaks in the q_2 -direction are clearly visible.

Figure 9(d) shows the scattering intensity for the case with the geometrically necessary dislocations along with the random distribution of dislocations shown in figure 8(d). The scattering is not concentrated along the q_1 - or q_2 -axes, but it is smeared out in the plane. In this scattering distribution the peaks seen in figure 9(b) have been masked due to the scattering from the randomly distributed dislocations. Since there are about three times as many randomly distributed dislocations (320/cell) as dislocations in the pile-up (90/cell) the dominant contribution comes from the randomly distributed dislocations.

Using the scattering intensities for the idealized distributions just derived we can now proceed to understand the features of the scattering intensities that were obtained from the dislocation dynamics simulations shown in figure 7. For the scattering from material (i), the two strong bands at $q_1 = \pm\pi/w$ in figure 7(a) are indeed consistent with the predictions

Figure 9. Small-angle scattering intensities for the idealized dislocation configurations structures in figure 8. (a) For the dislocation carpet configuration in figure 8(a). (b) For the array of geometrically necessary dislocations along the boundary between the reinforcement and the matrix in figure 8(b). (c) For the configuration in figure 8(c). (d) For the configuration of geometrically necessary and statistical dislocations in figure 8(d). The scattering intensities were computed by assuming that the dislocation distributions are repeated periodically in the matrix material. Image fields are not included. The scale is as shown in figure 7.

of scattering intensity for the idealized dislocation carpet structure of figure 8(a) shown in figure 9(a). However, the other peaks are replaced by a more complicated pattern. This feature may be understood by noticing that while we have assumed a well ordered dislocation structure in figure 8(a), the actual structure from the dislocation dynamics simulations, figure 4(a), are not perfectly ordered. Furthermore, the scattering from the image fields also leads to a deviation from the idealized situation.

Although material (iii) displays a rather complicated scattering pattern, figure 7(b), it has features of the idealized distributions considered in figures 8(b)–8(d), superimposed on a strong random background. For example, peaks along the q_2 -axis are the signatures of slip bands, while the peak-like features in the q_1 -direction allow connection with the geometrically necessary dislocations. However, the strong random background as well the presence of the image fields partially suppresses some of these peaks.

4.3. Continuum plasticity theory

The parameters entering (13) are taken to be: $h_0/\mu = 2.47 \times 10^{-4}$; $\gamma_0 = 0.002$; $N = 1.0$ or $N = 0.3$; $\ell = 0$ ($c/\ell = \infty$) or $\ell = 10 \mu\text{m}$ ($c/\ell = 0.1$) and $p = 0.5$. In addition, the initial value of the hardness g_0 is given by $g_0/\mu = 1.33 \times 10^{-3}$ and the strain-rate sensitivity parameters in (11) are specified as $\dot{\gamma}_0 = 0.002 \text{ s}^{-1}$ and $m = 0.005$. In [25] these parameters were found to give a good representation of the overall shear stress versus shear strain response for both material (i) and material (iii).

The deformed mesh for material (i) in figure 10(a) for the non-local theory with $N = 1$ and $c/\ell = 0.1$ shows that deformation concentrates in the vein between particles, but not to the same localized extent as the discrete dislocation prediction, figure 5(a). Even the local theory ($c/\ell = \infty$) does not predict a localized shear band, because the material is taken to be strain hardening. On the other hand, for material (iii), in figure 10(b) the dominant feature of the rotation of the centre reinforcement.

Figure 11 shows contours of constant dilation, $\epsilon_{ii} = u_{i,i}$ in the reference configuration for the non-local continuum plasticity calculations for materials (i) and (iii) with $c/\ell = 0.1$ and $N = 1.0$. For material (i), in figure 11(a), the dilation is small and positive in the first and third quadrants and small and negative in the second and fourth quadrants. With the prominent exception of the lack of the narrow band due to the dislocation carpet structure, the dilation distribution in figure 11(a) is similar to that in figure 6(a). However, here the corners of the reinforcements give rise to small positive and negative dilations. The overall dilation distribution for material (iii) in figure 11(b) corresponds quite well with that in figure 6(b), especially the rectangular bands in between neighbouring particles. There are significant differences in dilation, however, above and below the central particle as well as stemming from the local effects of the discrete dislocations.

Figure 12 shows the scattering intensities for material (i). The cases with $c/\ell = \infty$ correspond to the predictions of the classical local continuum plasticity theory. Comparing the scattering intensities in figure 12 with those in figure 7(a), the absence of the high intensity along the q_2 -axis is evident. This feature in figure 7(a) is a consequence of the dislocations in the rather narrow dipolar carpet. It is of interest to note that the closest resemblance to the discrete dislocation scattering intensities for material (i) is obtained for $N = 1.0$ and $c/\ell = 0.1$. On the other hand, this high hardening and strong non-locality act to suppress shear localization, which is contrary to the slip band observations in figure 5(a).

The scattering intensities for material (iii) are shown in figure 13. The overall scattering intensities are much larger for material (iii) than for material (i), which is expected from the dilation contours in figure 11. Qualitatively, the overall structure of the scattering amplitudes

Figure 10. Deformed meshes computed using non-local continuum plasticity with $N = 1.0$ and $c/\ell = 0.1$: (a) material (i) at $\Gamma = 0.58\%$. (b) material (iii) $\Gamma = 0.96\%$. The displacements are multiplied by a factor of 10.

for the continuum plasticity calculations in this case are the same as for the discrete dislocation calculation in figure 7(b), with the exception of a less intense background for continuum plasticity. This is expected since the dilation fields are similar except for effects associated with individual discrete dislocations. There are some differences in the scattering pattern between the local ($c/\ell = \infty$) and non-local material descriptions. For the local material, figures 13(a) and 13(c), there are strong peaks in the q_1 -direction spaced at about $6 \mu\text{m}^{-1}$, while the peaks in the q_2 -direction are less resolved. On the other hand, in the non-local models the intensity is more concentrated along the q_2 -direction than along the q_1 -direction. The peak spacing in the q_2 -direction of roughly $20 \mu\text{m}^{-1}$ corresponds to the height of the horizontal band of high dilation between particles seen in figure 11. Comparison with the idealized dislocation structure with both the dipolar carpet as well as the geometrically necessary dislocations in figure 9(c) allows us to identify this spacing of the peaks in the q_2 -direction with the height of the horizontal dilation band ($0.33 \mu\text{m}$). The closest agreement with the discrete dislocation results is obtained using $N = 1.0$ and $c/\ell = 0.1$.

Figure 11. Contours of $u_{i,i}$ computed using non-local continuum plasticity with $N = 1.0$ and $c/\ell = 0.1$: (a) material (i) at $\Gamma = 0.58\%$ and (b) material (iii) at $\Gamma = 0.96\%$.

Contours of the non-vanishing component of Nye's dislocation density tensor are shown in figure 14 for $N = 1.0$ and $c/\ell = 0.1$ for both material (i) and material (iii). For material (i) the main gradient in slip is in the x_2 -direction and, since $\alpha_{13} = \partial\gamma/\partial x_1$, the values of α_{13} are fairly uniform except near the corners of the reinforcements. The concentration of α_{13} along the sides of the central particle for material (iii) is qualitatively consistent with the existence of the geometrically necessary dislocations seen in figure 4. Bassani *et al* [25] note that for material (iii) the distributions of α_{13} obtained from non-local plasticity theory tend to be smoother than predicted by the local theory, due to gradient hardening. On the other hand, there is little difference between the predictions of the local and non-local theories for material (i).

The small-angle scattering patterns computed from the dislocation densities in figure 14 are shown in figure 15. These scattering patterns exhibit some of the features of the scattering

Figure 12. Small-angle scattering amplitudes for the continuum plasticity simulations of material (i) at $\Gamma = 0.58\%$: (a) $N = 0.3$, $c/\ell = \infty$; (b) $N = 0.3$, $c/\ell = 0.1$; (c) $N = 1.0$, $c/\ell = \infty$; and (d) $N = 1.0$, $c/\ell = 0.1$. The scale is as shown in figure 7.

Figure 13. Small-angle scattering amplitudes for the continuum plasticity simulations of material (iii) at $\Gamma = 0.96\%$: (a) $N = 0.3$, $c/\ell = \infty$; (b) $N = 0.3$, $c/\ell = 0.1$; (c) $N = 1.0$, $c/\ell = \infty$; and (d) $N = 1.0$, $c/\ell = 0.1$. The scale is as shown in figure 7.

Figure 14. Contours of the non-vanishing component of Nye's dislocation density tensor, $\alpha_{13} = \partial\gamma/\partial x_1$ (μm^{-1}), computed using non-local continuum plasticity with $N = 1.0$ and $c/\ell = 0.1$: (a) material (i) at $\Gamma = 0.58\%$ and (b) material (iii) at $\Gamma = 0.96\%$.

intensities in figures 12 and 13. However, a key difference between the scattering patterns based on the discrete dislocation analysis and the predictions of the non-local theory of Acharya and Bassani [9] is that in the non-local continuum results the density of geometrically necessary dislocations is smeared out. This is seen in particular for material (iii) on the sides of the central reinforcing particle in figure 14(b). As a result of the smearing out the dislocation density in real space, the scattering intensity in $\mathbf{q}$ space tends to be localized around the origin. In figure 15(b) there is very little scattering intensity for $q_1 > 0$. For material (i), the scattering pattern in figure 15(a) is similar to the central features exhibited in figure 12(d), but here too the amplitude at large $\mathbf{q}$ values is smaller.

Figure 15. Small-angle scattering amplitudes computed from (35) using the distributions of Nye's dislocation density tensor in figure 14: (a) material (i) at $\Gamma = 0.58\%$ and (b) material (iii) at $\Gamma = 0.96\%$. The scale is as shown in figure 7.

5. Concluding remarks

Small-angle scattering patterns clearly distinguish between different dislocation structures. Within the framework of a two-dimensional model material we find that walls of geometrically necessary dislocations give rise to a distinctly different scattering pattern from that which is obtained for a carpet of dislocations arising from localized slip. Characteristic sizes of these structures can be identified from the spacings of the peaks in the scattering intensities.

Although the simulations clearly show that the dislocation structures resulting from plastic deformation can be identified by small-angle scattering, it is important to remember that plastic deformation is the consequence of the slip motion of these dislocations. Hence, in order to quantify the plastic deformation the dislocation motion must be known. This is a fundamental issue in the link between dislocation scattering patterns and plastic deformation.

Relatively simple continuum models of plastic deformation have been shown to be capable of picking up some of the important features of the scattering patterns. Local features that are due to the individual dislocations are evidently missing. This is also true for the non-local plasticity theory considered here, even though this theory is able to account, in a phenomenological sense, for some effects of geometrically necessary dislocations related to strain gradients on the overall response [25].

The analyses have been based on a model composite material that gives rise to ordered dislocation structures in the discrete dislocation simulations. The difference in scattering properties between the matrix and the reinforcement has been ignored. In a real composite, the difference in electron density between the matrix and the reinforcement would mask the scattering patterns due to the dislocations structure. Also, a real material will not exhibit the periodicity assumed in the present computations. Therefore, it remains to be seen whether or not the distinctly different scattering patterns associated with various organized dislocation structures can be discerned in real materials.

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