A comparison of dislocation induced back stress formulations in strain gradient crystal plasticity

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Abstract

Strain gradient crystal plasticity attempts to predict material size effects by taking into account geometrically necessary dislocations that are required to accommodate gradients of crystallographic slip. Since these dislocations have a non-zero net Burgers vector within the material, dislocation induced long range stresses result in a back stress that influences the effective driving force for crystallographic slip. A dislocation induced back stress formulation is proposed in which the full tensorial nature of the dislocation stress state is included in the continuum description. The significance of this proposed back stress formulation is that it intrinsically includes latent kinematic hardening from dislocations lying on all slip systems. Using simple shearing of a semi-infinite cube oriented single crystal with either double-planar or octahedral slip system configurations, the proposed back stress formulation is examined in detail.

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1. Introduction

Strain gradient crystal plasticity formulations which include geometrically necessary dislocations have been developed in the past years by a number of researchers, for example by Han et al. (2005a), Han et al. (2005b), Yefimov et al. (2004), Yefimov and Van der Giessen (2005), Evers et al. (2004a,b) and Gurtin (2002). The various models have been applied to study length scale effects in crystalline materials which have been experimentally observed by Motz et al. (2005), Stölken and Evans (1998) and Fleck et al. (1994). In these experiments macroscopic length scale effects were observed whereby the specimen dimensions influence the constitutive response of the material, while at the microstructural level, material size effects are observed as the grain size dependence of the flow stress. These experimental results cannot be predicted using conventional
plasticity formulations since they fail to capture the strain gradients associated with the geometrical necessary dislocations (GNDs), which are required to ensure lattice compatibility, see Ashby (1970). Furthermore the crystal plasticity models enable the proper incorporation of the anisotropy of the crystallographic slip and the nature of the granular polycrystals.

While the above gradient based plasticity formulations employ different concepts and methods to estimate the GND densities, a common feature is the use of dislocation governed hardening rules rather than phenomenological based hardening rules to determine the slip system resistance. These models therefore have the advantage of including a more physically motivated approach to determine the crystallographic slip resistance based on the interaction of dislocations on different slip systems. While the GND densities are directly incorporated within the slip system resistance, back stresses associated with the second order strain gradients are occasionally included in the constitutive model as shown by Yefimov et al. (2004), Yefimov and Van der Giessen (2005) and Evers et al. (2004a,b) to capture size dependent effects. However, Han et al. (2005a,b) demonstrated for the cases of micro-bending, simple shear and a bar subjected to a constant body force, that size dependent effects can also be captured with only first order strain gradients incorporated within the strengthening term. In the present strain gradient crystal plasticity formulation, size effects are captured through both the slip system resistance term \( s^a \) in a similar fashion as Han et al. (2005a), and through the introduction of a dislocation induced back stress term \( \tau_b^a \). In the present model, the back stresses resulting from the dislocation induced internal stresses dominate the size effect predictions.

While the stress states associated with individual dislocations are well understood, the continuum description of an internal stress tensor associated with these dislocations lying on a number of slip systems has remained an open issue. Inspired by this challenge, a novel dislocation induced internal stress formulation is proposed in which the internal stress tensor is determined from the stresses associated with the dislocation gradients on all slip systems. It differs from the back stress formulations proposed by Evers et al. (2004a,b), Yefimov et al. (2004) and Yefimov and Van der Giessen (2005) since the back stress on each individual slip system includes not only the dislocation induced stress components acting on that slip system, but also the full tensorial nature of the stress contribution arising from dislocations on all other slip systems as well. Therefore the proposed formulation is a continuum tensorial description of the dislocation induced stress field that intrinsically combines latent kinematic hardening effects from dislocations lying on all slip systems.

This paper aims to elucidate the differences between the two above mentioned internal stress formulations and to compare their predictions for simple shear of a semi-infinite block of material for the cases of double-planar and octahedral slip of an FCC single crystal.

2. Gradient crystal plasticity with dislocation governed hardening

2.1. Strain gradient crystal plasticity

The strain gradient crystal plasticity model adopted from Evers et al. (2004a,b), is briefly described along with its numerical implementation. A key feature of the model is the incorporation of both geometrically necessary (GND) and statistically stored (SSD) dislocation densities which are used to describe the crystallographic slip resistance, while the gradients of the GNDs are used to determine the dislocation induced back stress.

In order to consistently represent the different scalar, vector and tensorial quantities, the following convention is adopted: scalar quantities are written in italic letters i.e. \( y_c \), vectorial quantities are written in bold italics i.e. \( s^a \) and \( n^a \), and matrices and second tensors are written in an upright sans-serif font i.e. \( F_e \) and \( S \), while fourth order tensors are expressed as \( C \). Tensorial notation is used throughout whereby \( \cdot \) represents an inner product and \( : \) represents the double inner product.

As a classical point of departure, the deformation gradient tensor \( F \), is multiplicatively decomposed into its elastic part \( F_e \) and a plastic part \( F_p \), which is visualized in Fig. 1, according to:

\[
F = F_e \cdot F_p
\]  

The plastic contribution \( F_p \) refers to the deformation from the initial reference configuration to the intermediate stress-free configuration. This stress-free configuration is considered to develop from the reference configuration solely by plastic shearing along the active slip planes of the crystal lattice through crystallographic
slip, and thus leaves the orientations of the slip systems unaltered. The elastic part of the deformation tensor rotates and stretches the plastically deformed lattice into the current configuration.

In Fig. 1, an arbitrary slip system is labeled by a superscript \( z \), with \( z = 1, 2, \ldots, n_s \) where \( n_s \) is the total number of slip systems defined according to Table 1 for an FCC crystal. In the reference state, a slip system \( z \) is identified by unit vectors representing the slip plane normal \( \mathbf{n}_0^z \) and the associated slip direction \( \mathbf{s}_0^z \), which is perpendicular to \( \mathbf{n}_0^z \).

The plastic velocity gradient tensor in the intermediate configuration \( \mathbf{L}_p \) is composed of the contributions over the slip systems:

\[
\mathbf{L}_p = \sum_{z=1}^{n_s} \dot{\gamma}^z \mathbf{s}_0^z \mathbf{n}_0^z
\]

where the summation runs over the total number \( n_s \) of slip systems and where \( \dot{\gamma}^z \) is the yet to be defined slip rate quantity on each individual slip system \( z \). The plastic velocity gradient tensor is related to the plastic deformation gradient tensor according to:

**Table 1**

<table>
<thead>
<tr>
<th>( \zeta )</th>
<th>( z )</th>
<th>Dislocation type</th>
<th>( \mathbf{n}_0^z )</th>
<th>( \mathbf{s}_0^z )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>Edge</td>
<td>( \frac{1}{\sqrt{2}}[110] )</td>
<td>( \frac{1}{\sqrt{2}}(111) )</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>Edge</td>
<td>( \frac{1}{\sqrt{2}}[101] )</td>
<td>( \frac{1}{\sqrt{2}}(111) )</td>
</tr>
<tr>
<td>3</td>
<td>3</td>
<td>Edge</td>
<td>( \frac{1}{\sqrt{2}}[011] )</td>
<td>( \frac{1}{\sqrt{2}}(111) )</td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td>Edge</td>
<td>( \frac{1}{\sqrt{2}}[110] )</td>
<td>( \frac{1}{\sqrt{2}}(111) )</td>
</tr>
<tr>
<td>5</td>
<td>5</td>
<td>Edge</td>
<td>( \frac{1}{\sqrt{2}}[101] )</td>
<td>( \frac{1}{\sqrt{2}}(111) )</td>
</tr>
<tr>
<td>6</td>
<td>6</td>
<td>Edge</td>
<td>( \frac{1}{\sqrt{2}}[011] )</td>
<td>( \frac{1}{\sqrt{2}}(111) )</td>
</tr>
<tr>
<td>7</td>
<td>7</td>
<td>Edge</td>
<td>( \frac{1}{\sqrt{2}}[110] )</td>
<td>( \frac{1}{\sqrt{2}}(111) )</td>
</tr>
<tr>
<td>8</td>
<td>8</td>
<td>Edge</td>
<td>( \frac{1}{\sqrt{2}}[101] )</td>
<td>( \frac{1}{\sqrt{2}}(111) )</td>
</tr>
<tr>
<td>9</td>
<td>9</td>
<td>Edge</td>
<td>( \frac{1}{\sqrt{2}}[011] )</td>
<td>( \frac{1}{\sqrt{2}}(111) )</td>
</tr>
<tr>
<td>10</td>
<td>10</td>
<td>Edge</td>
<td>( \frac{1}{\sqrt{2}}[110] )</td>
<td>( \frac{1}{\sqrt{2}}(111) )</td>
</tr>
<tr>
<td>11</td>
<td>11</td>
<td>Edge</td>
<td>( \frac{1}{\sqrt{2}}[101] )</td>
<td>( \frac{1}{\sqrt{2}}(111) )</td>
</tr>
<tr>
<td>12</td>
<td>12</td>
<td>Edge</td>
<td>( \frac{1}{\sqrt{2}}[011] )</td>
<td>( \frac{1}{\sqrt{2}}(111) )</td>
</tr>
<tr>
<td>13</td>
<td>4 or 7</td>
<td>Screw</td>
<td>( \frac{1}{\sqrt{2}}[110] )</td>
<td>( \frac{1}{\sqrt{2}}(111) ) or ( \frac{1}{\sqrt{2}}(111) )</td>
</tr>
<tr>
<td>14</td>
<td>5 or 11</td>
<td>Screw</td>
<td>( \frac{1}{\sqrt{2}}[101] )</td>
<td>( \frac{1}{\sqrt{2}}(111) ) or ( \frac{1}{\sqrt{2}}(111) )</td>
</tr>
<tr>
<td>15</td>
<td>9 or 12</td>
<td>Screw</td>
<td>( \frac{1}{\sqrt{2}}[011] )</td>
<td>( \frac{1}{\sqrt{2}}(111) ) or ( \frac{1}{\sqrt{2}}(111) )</td>
</tr>
<tr>
<td>16</td>
<td>1 or 10</td>
<td>Screw</td>
<td>( \frac{1}{\sqrt{2}}[110] )</td>
<td>( \frac{1}{\sqrt{2}}(111) ) or ( \frac{1}{\sqrt{2}}(111) )</td>
</tr>
<tr>
<td>17</td>
<td>2 or 8</td>
<td>Screw</td>
<td>( \frac{1}{\sqrt{2}}[101] )</td>
<td>( \frac{1}{\sqrt{2}}(111) ) or ( \frac{1}{\sqrt{2}}(111) )</td>
</tr>
<tr>
<td>18</td>
<td>3 or 6</td>
<td>Screw</td>
<td>( \frac{1}{\sqrt{2}}[011] )</td>
<td>( \frac{1}{\sqrt{2}}(111) ) or ( \frac{1}{\sqrt{2}}(111) )</td>
</tr>
</tbody>
</table>
\[ \mathbf{F}_p = \mathbf{L}_p \cdot \mathbf{F}_p \] (3)

The elastic behaviour is considered with respect to the fictitiously unloaded configuration defined by the plastic deformation gradient tensor \( \mathbf{F}_p \). A hyper-elastic formulation is selected where the second Piola–Kirchhoff stress tensor \( \mathbf{S} \) is expressed in the (elastic) Green–Lagrange strain tensor \( \mathbf{E}_e \) defined in the current state with respect to the intermediate configuration according to:

\[ \mathbf{S} = \mathbf{C} : \mathbf{E}_e \quad \text{with } \mathbf{E}_e = \frac{1}{2} (\mathbf{F}_e^T \cdot \mathbf{F}_e - \mathbf{I}) \] (4)

with \( \mathbf{I} \) the second order identity tensor, while the stress tensor \( \mathbf{S} \) is defined by

\[ \mathbf{S} = \mathbf{F}_e^{-1} \cdot \mathbf{\tau} \cdot \mathbf{F}_e^{-T} \quad \text{with } \mathbf{\tau} = \mathbf{J}_e \sigma \] (5)

with \( \mathbf{\tau} \) the Kirchhoff stress tensor; \( \sigma \), the Cauchy stress tensor and \( \mathbf{J}_e = \det(\mathbf{F}_e) = \det(\mathbf{F}) \), the volume change ratio while for \( \mathbf{C} \) the fourth order isotropic elasticity tensor is taken.

For a given slip system \( \alpha \) the resolved shear stress \( \tau^{\alpha} \) (also called the Schmid stress) in the intermediate state can be determined through:

\[ \tau^{\alpha} = s_0^{\alpha} \cdot \mathbf{S} \cdot n^{\alpha} \] (6)

The connection between the single crystal kinematics and the underlying dislocation density development is accomplished through a visco-plastic power-law which relates the slip rates to the effective shear stress \( \tau^{\alpha}_{\text{eff}} \) and the slip system resistance \( s^{\alpha} \) according to:

\[ \dot{\tau}^{\alpha} = \dot{\gamma}_0 \left( \frac{|\tau^{\alpha}_{\text{eff}}|}{s^{\alpha}} \right)^{1/m} \exp \left[ -\frac{G_0}{kT} \left( 1 - \frac{|\tau^{\alpha}_{\text{eff}}|}{s^{\alpha}} \right) \right] \text{sign}(\tau^{\alpha}_{\text{eff}}) \] (7)

with \( \dot{\gamma}_0 \) and \( m \) material parameters, representing the reference plastic shear rate and the rate sensitivity, respectively. \( T \) and \( k \) are the absolute temperature and Boltzmann’s constant, respectively, and \( G_0 \) is the thermal activation energy necessary to activate dislocation motion. With a large value of \( m \) (i.e. \( m = 10 \)) \( \dot{\gamma}^{\alpha} \) remains negligible unless \( |\tau^{\alpha}_{\text{eff}}| \) is close to \( s^{\alpha} \) or larger.

The effective shear stress \( \tau^{\alpha}_{\text{eff}} \) constitutes the driving force for crystallographic slip through dislocation motion on slip system \( \alpha \) and is determined as the difference between the externally imposed resolved shear stress \( \tau^{\alpha} \) and the yet to be defined resolved back stress \( \tau^{\alpha}_b \) according to:

\[ \tau^{\alpha}_{\text{eff}} = \tau^{\alpha} - \tau^{\alpha}_b \] (8)

The slip system resistance \( (s^{\alpha}) \) is a measure of the impedance of dislocation motion on the slip systems by the formation of short-range interactions between all dislocations. Physically dislocations are discrete loops but are represented here by a continuous field of dislocations with either an edge or screw nature. In contrast to more phenomenological crystal plasticity models which relate the slip resistance to the history of the plastic shear on all slip systems, here the slip resistance \( s^{\alpha} \) on slip system \( \alpha \) is expressed as a function of both the dislocation densities \( \rho^{\alpha}_{\text{GND}} \) and \( \rho^{\alpha}_{\text{SSD}} \), with the superscript \( \xi \) denoting the dislocation type as labeled in Table 1. The slip system resistance includes the contribution of both the SSDs and GNDs according to:

\[ s^{\alpha} = Gb \sqrt{\sum_{\xi=1}^{12} A^{\alpha \xi} \rho^{\alpha \xi}_{\text{SSD}}} + \sum_{\xi=1}^{18} A^{\alpha \xi} \rho^{\alpha \xi}_{\text{GND}}} \] for \( \alpha = 1, 2, \ldots, n_s \) (9)

where \( G \) is the shear modulus, \( b \) is the magnitude of the Burgers vector, and \( A^{\alpha \xi} \) is a component of an interaction matrix which represents the strength of the interactions between slip systems as defined by Franciosi and Zouoi (1982). The six interaction coefficients corresponding to self hardening, coplanar, Hirth lock, glissile junction, Lomer Cottrell lock, and cross slip are further defined in Arsenlis and Parks (2002). It should be noticed that in Eq. (9), only edge SSDs participate in the slip resistance while for the GNDs both the edge and screw dislocations are taken into account.
2.2. Internal stress formulations

Because dislocations disturb the regularity of crystal lattices they constitute a source of internal stress. For statistically stored dislocations, which usually have a random orientation, the net internal stress contribution will be self-equilibrating. However, geometrically necessary dislocations may cause a significant internal stress state, which can be estimated from the elastic stress associated with individual (denoted with the superscript ind) edge and screw dislocations $\sigma_{\text{edge}}^{\text{ind}}$, $\sigma_{\text{screw}}^{\text{ind}}$, respectively, in an infinite medium.

For an individual screw dislocation located at the origin of a coordinate system as defined in Fig. 2a, the full internal dislocation induced stress state is expressed by Cottrell (1952), using small deformation theory as

$$
\begin{align*}
\sigma_{xx}^{\text{ind}} &= 0, \quad \sigma_{xy}^{\text{ind}} = 0 \\
\sigma_{yy}^{\text{ind}} &= 0, \quad \sigma_{xz}^{\text{ind}} = -\frac{G b}{2\pi} \frac{y}{x^2 + y^2} \\
\sigma_{zz}^{\text{ind}} &= 0, \quad \sigma_{yz}^{\text{ind}} = 0
\end{align*}
$$

while for the edge dislocation shown in Fig. 2b, the full internal dislocation induced stress state can be described as

$$
\begin{align*}
\sigma_{xx}^{\text{ind}} &= -\frac{G b}{2\pi(1-v)} \frac{y(3x^2 + y^2)}{(x^2 + y^2)^2}, \quad \sigma_{xy}^{\text{ind}} = \frac{G b}{2\pi(1-v)} \frac{x(x^2 - y^2)}{(x^2 + y^2)^2} \\
\sigma_{yy}^{\text{ind}} &= \frac{G b}{2\pi(1-v)} \frac{y(x^2 - y^2)}{(x^2 + y^2)^2}, \quad \sigma_{xz}^{\text{ind}} = 0 \\
\sigma_{zz}^{\text{ind}} &= -\frac{G b v}{\pi(1-v)} \frac{y}{x^2 + y^2}, \quad \sigma_{yz}^{\text{ind}} = 0
\end{align*}
$$

where $v$ is Poisson’s ratio. These equations, with opposite signs, also provide the stress in the origin of the coordinate system for a dislocation located in the position $(x,y)$.

From these dislocation induced stress fields, two back stress formulations are derived here which differ in the number of participating stress components. The self-internal back stress formulation assumes that only the shear stress components acting on the $\xi$ slip system, i.e. $\sigma_{xz}^{\text{ind}}$ for the screw dislocations and $\sigma_{xy}^{\text{ind}}$ for the edge dislocations, obstruct dislocation motion since they lie on that slip system. This internal stress formulation is the one considered by Evers et al. (2004a,b) and is similar to the self-back stress formulation proposed by Yefimov and Van der Giessen (2005). By considering not only the dislocation induced stresses acting on the slip system, but the complete stress tensor, a continuum internal stress tensor is proposed and is subsequently termed the full internal stress formulation.

Within a uniform field of dislocations, dislocations positioned equidistant from the origin would have associated opposed stress values according to Eqs. (10) and (11) and would therefore not contribute to the internal stress. For this reason only the gradients of the dislocation field contributes to the net internal stress.

![Fig. 2. Individual screw (a) and edge (b) dislocations defining the coordinate system used to calculate the dislocation induced internal stress field.](image)
Since dislocation fields rather than individual dislocations are considered, the number of \( z \) oriented dislocations per unit area in the \( xy \)-plane can be obtained by a first-order approximation through:

\[
\rho_{\text{GND}}(x, y) = \rho_{\text{GND}0} + \frac{\partial \rho_{\text{GND}}}{\partial x} x + \frac{\partial \rho_{\text{GND}}}{\partial y} y
\]  (12)

with \( \rho_{\text{GND}0} \) and the partial derivatives of \( \rho_{\text{GND}} \) taken at the origin. Note that Eq. (12) in fact constitutes a truncated Taylor series expansion of the continuous dislocation field. It naturally implies a separation of scales, since it assumes a linear variation of the dislocation density in a bounded region. Only dislocations within a circular domain of radius \( R \) satisfying \( x^2 + y^2 \leq R^2 \) are assumed to contribute to the internal stress field. Dislocations at a larger distance than \( R \) do not participate since the linearization assumed in Eq. (12) would no longer be valid. Rewriting Eqs. (10) and (12) in cylindrical coordinates, followed by analytical integration over the circular domain, the internal stress state at the origin associated with a field of screw dislocations can be expressed as

\[
\sigma_{xx} = 0, \quad \sigma_{xy} = 0 \]
\[
\sigma_{yy} = \frac{GbR^2}{4} \frac{\partial \rho}{\partial y}, \quad \sigma_{xz} = \frac{GbR^2}{4} \frac{\partial \rho}{\partial x} \]
\[
\sigma_{zz} = 0, \quad \sigma_{zz} = -\frac{GbR^2}{4} \frac{\partial \rho}{\partial x}
\]  (13)

Similarly for a distributed field of \( z \) oriented edge dislocations, analytical integration of the stress due to individual dislocations over the domain \( R \) yields:

\[
\sigma_{xx} = \frac{3GbR^2}{8(1-v)} \frac{\partial \rho}{\partial y}, \quad \sigma_{xy} = -\frac{GbR^2}{8(1-v)} \frac{\partial \rho}{\partial x} \]
\[
\sigma_{yy} = \frac{GbR^2}{8(1-v)} \frac{\partial \rho}{\partial y}, \quad \sigma_{xz} = 0
\]
\[
\sigma_{zz} = \frac{GbR^2}{2(1-v)} \frac{\partial \rho}{\partial y}, \quad \sigma_{yz} = 0
\]  (14)

When (13) and (14) are reformulated taking into account the crystallographic axes in the intermediate configuration, the full internal stress associated with a screw dislocation field can be expressed as

\[
\sigma_{s}^{\text{int}} = \frac{GbR^2}{4} \sum_{i=1}^{18} \nabla \rho_{\text{GND}} \left[ \begin{array}{c}
- n_i^{s} s_i^{p} \delta_{yx} - n_i^{s} p_i^{p} \delta_{xy} + p_i^{s} s_i^{p} \delta_{xz} + p_i^{s} n_i^{p} \delta_{zx} + p_i^{s} m_i^{p} \delta_{yz} - s_i^{s} m_i^{p} \delta_{zy} - s_i^{s} n_i^{p} \delta_{yx} - n_i^{s} p_i^{p} \delta_{xy}
\end{array} \right]
\]  (15)

while for a field of edge dislocations, the full internal stress can be rewritten as

\[
\sigma_{e}^{\text{int}} = \frac{GbR^2}{8(1-v)} \sum_{i=1}^{12} \nabla \rho_{\text{GND}} \left[ \begin{array}{c}
3 n_i^{e} s_i^{p} s_i^{p} + n_i^{e} s_i^{p} m_i^{p} + 4 m_i^{e} p_i^{p} p_i^{p} - s_i^{e} s_i^{p} p_i^{p} - s_i^{e} n_i^{p} n_i^{p} - s_i^{e} m_i^{p} b_i^{p} - s_i^{e} n_i^{p} b_i^{p}
\end{array} \right]
\]  (16)

where \( n_i^{s} \) and \( s_i^{s} \) define the slip system normal and slip direction, \( \delta_{xy} = s_i^{s} \times n_i^{s} \) associated with the \( \zeta \) dislocation listed in Table 1. The indications below the underbraces identify the relevant stress components for a \( z \) oriented dislocation whose coordinates are given in Fig. 2 for screw and edge dislocations, respectively. For the screw dislocations, \( \text{either} \) one of the two slip systems defined in Table 1 results in an equivalent internal stress, and therefore the choice of slip system associated with the screw dislocation is irrelevant.

From the above specification of the internal stress formulations, the self-internal formulation considers only the stress components capable of causing dislocation motion on the \( \zeta \) slip system. For a screw dislocation this is limited to only the \( yz \) and \( xy \) terms, while for an edge dislocation only the \( xy \) and \( yx \) terms are included, and thus for the self-internal stress formulation equations (15) and (16) become:
\[
\sigma_s^{\text{int}} = \frac{G b R^2}{4} \sum_{\xi=13}^{18} \nabla_0 \rho_{GND}^\xi \cdot \left[ p_{\xi}^0 n_{0}^\xi \frac{n_{y}^\xi}{y} + p_{\xi}^0 n_{0}^\xi \frac{n_{y}^\xi}{y} \right]
\]

for a field of screw dislocations while for a field of edge dislocations, the self-internal stress can be rewritten as

\[
\sigma_e^{\text{int}} = \frac{G b R^2}{8 (1 - \nu)} \sum_{\xi=1}^{12} \nabla_0 \rho_{GND}^\xi \cdot \left[ -s_0^\xi n_0^\xi \frac{n_{y}^\xi}{y} - s_0^\xi n_0^\xi \frac{n_{y}^\xi}{y} \right]
\]

Analogous to resolving the Schmid stress on each slip system defined in Eq. (6), the back stress on each slip system is related to the dislocation induced internal stress according to:

\[
\tau_b^\xi = -s_0^\xi \cdot (\sigma_s^{\text{int}} + \sigma_e^{\text{int}}) \cdot n_0^\xi
\]

where the minus sign in the right-hand side of Eq. (19) is introduced to represent the so-called slip obstructing character of the back stress. Latent hardening, herein defined as the hardening on a secondary slip system caused by dislocation gradients on a primary slip system, is incorporated by summation over \(n = 1, 2, 3, \ldots, 12\) for the edge dislocations and \(n = 13, 14, \ldots, 18\) for the screw dislocations, respectively. Since the full internal stress tensor contains the out-of-plane stress terms associated with each \(\xi\) dislocation type, it differs from the one obtained from the self-internal formulation and leads to significantly different resolved back stresses as will be discussed in Section 6.1.

3. Dislocation density evolution

3.1. SSDs

The evolution of the 12 edge SSD densities of an FCC material, which are required for Eq. (9), is based on the balance between accumulation and annihilation rates according to (Harder, 1999; Arsenlis and Parks, 2002; Evers et al., 2004a,b):

\[
\dot{\rho}_{SSD}^\xi = \frac{1}{b} \left( \frac{1}{L_\xi} - 2 y_c \frac{\rho_{SSD}^\xi}{\rho_{SSD}} \right) |y_c^\xi| \quad \text{with} \quad \rho_{SSD}(t = 0) = \rho_{SSD_0}
\]

The accumulation rate (first term in the right-hand side of Eq. (20)) is governed by the average dislocation segment length of mobile dislocations (SSDs) on system \(\xi\), denoted by \(L_\xi^*\), which is strongly related to the current dislocation state according to:

\[
L_\xi^* = \frac{K}{\sqrt{\sum_{\xi=1}^{12} H^\xi |\rho_{SSD}^\xi| + \sum_{\xi=1}^{18} H^\xi |\rho_{GND}^\xi|}}
\]

In this expression the dimensionless coefficients \(H^\xi\), represent the mutual immobilization between dislocations of different slip systems, and are structured analogously to the coefficients \(A^\xi\) introduced in Eq. (9), however, the values are generally different (see Table 2). Furthermore, the annihilation rate (second term in the right-hand side of Eq. (20)) is assumed to be controlled by the critical annihilation length \(y_c\), a material parameter characterizing the average distance between dislocations of opposite signs which triggers spontaneous neutralization. Note that Eq. (20) does not imply that GNDs are not mobile. Individual dislocations cannot discriminate between being SSD or GND. In fact, the GND fraction of the total dislocation population is determined geometrically and not through (20). Nevertheless, GNDs do contribute in the production of dislocations, as clearly emphasized in Eq. (21).

3.2. GNDs

Gradients in the plastic deformation within crystalline materials give rise to so-called geometrically necessary dislocations in order to maintain lattice continuity in the crystals. With the knowledge of the crystalline
orientation in relation to the plastic deformation gradient, the type of dislocation needed to preserve this continuity can be determined.

Considering one of the slip systems, it is obvious that only slip gradients in the plane of the slip system give rise to an incompatibility that will lead to GNDs. Slip gradients in the direction of the slip will be accommodated by edge dislocations while gradients in the slip plane perpendicular to the slip direction induce screw dislocations. The relationship between the gradient (with respect to the undeformed reference configuration) of the plastic slip $\gamma^a$ on a slip system $a$ (with $a = \xi = 1, 2, \ldots, 12$ for FCC material) and the associated edge GND density takes the following form (see Ashby, 1970):

$$\rho^\xi_{\text{GND}} = \rho^\xi_{\text{GND}_0} - \frac{1}{b} \nabla_0 \gamma^\xi \cdot s_0^\xi$$  \hspace{1cm} (22)

where an initial value of the GND density has been introduced to account for initially present geometrical lattice distortions (i.e. at small angle grain boundaries, see Evers et al. (2004b)). The screw GND densities for $\xi = 13, 14, \ldots, 18$, due to slip gradients can effectively be written as

$$\rho^\xi_{\text{GND}} = \rho^\xi_{\text{GND}_0} + \frac{1}{b} \left( \nabla_0 \gamma^{z_1} \cdot p_0^{z_1} + \nabla_0 \gamma^{z_2} \cdot p_0^{z_2} \right)$$  \hspace{1cm} (23)

with $z_1$ and $z_2$ indicating the two slip systems associated with each screw GND, which are listed in Table 1.

### 4. Finite element implementation

In order to systematically compute an approximate solution of the entire set of strongly non-linear and coupled equations for an arbitrary geometry and boundary condition, the previously described single crystal constitutive framework is implemented within the finite element method and solved at the integration point level. In order to model either single or polycrystalline deformations at the microstructural level, each integration point is chosen to represent a fraction of a single crystal, with aggregates of elements representing individual grains within the material.

As apparent from Eqs. (22) and (23) the spatial variation of the crystallographic slip throughout the domain is necessary to determine the GND densities, moreover, the evolution of the crystallographic slip rates (Eq. (7)) requires knowledge of the GND densities through the crystallographic resistance (Eq. (9)) and the internal stress (Eqs. (15) and (16)). However, if the GND densities and the spatial variation of the deformation are known, all relevant quantities can be determined. Therefore, the 18 GND densities are treated as nodal unknowns in a similar manner as the three displacements, increasing the number of nodal degrees of freedom to 21. These nodal unknowns are subsequently interpolated to the integration points through the element shape functions.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Magnitude</th>
<th>Used in equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$G$</td>
<td>Shear modulus</td>
<td>54.22 GPa</td>
<td>(9)-(11), (15), (16)</td>
</tr>
<tr>
<td>$v$</td>
<td>Poisson’s ratio</td>
<td>0.3278</td>
<td>(11), (16)</td>
</tr>
<tr>
<td>$b$</td>
<td>Burgers vector length</td>
<td>0.256 nm</td>
<td>(9)-(11) (15), (16), (20), (22), (23)</td>
</tr>
<tr>
<td>$K$</td>
<td>Disl. segment length constant</td>
<td>26.0</td>
<td>(21)</td>
</tr>
<tr>
<td>$\gamma_0$</td>
<td>Critical annihilation length</td>
<td>1.6 nm</td>
<td>(20)</td>
</tr>
<tr>
<td>$\rho_{\text{SSD0}}$</td>
<td>Initial SSD density</td>
<td>7.0 $\mu$m$^{-2}$</td>
<td>(20)</td>
</tr>
<tr>
<td>$R$</td>
<td>Disl. capture radius</td>
<td>0, 10, 25 $\mu$m</td>
<td>(15), (16)</td>
</tr>
<tr>
<td>$G_0$</td>
<td>Activation energy</td>
<td>4.54e$-20$ J</td>
<td>(7)</td>
</tr>
<tr>
<td>$k$</td>
<td>Boltzmann constant</td>
<td>1.38054e$-23$ J/K</td>
<td>(7)</td>
</tr>
<tr>
<td>$T_0$</td>
<td>Reference slip rate</td>
<td>$1 \times 10^{-3}$ s$^{-1}$</td>
<td>(7)</td>
</tr>
<tr>
<td>$m$</td>
<td>Rate sensitivity exponent</td>
<td>10</td>
<td>(7)</td>
</tr>
</tbody>
</table>

The magnitudes of the constants used for $A^{\xi\gamma}$ and $H^{\xi\gamma}$ are taken from Evers et al. (2004b).
As a point of departure to approximate the displacement and the GND density fields, the equilibrium and the GND densities versus slip gradients equations are taken for further elaboration. Equilibrium is formulated in terms of the first Piola–Kirchhoff stress tensor \( P \) related to the reference configuration defined as \( P = \det(F) \sigma \cdot F^{-T} \) according to:

\[
\nabla_0 \cdot P^T = 0
\]

(24)

assuming that distributed body forces can be omitted. Eqs. (22) and (23) for the GND densities are written in an abbreviated format as

\[
\rho_{\text{GND}}^\xi = \rho_{\text{GND}_0} + d_{\xi} \cdot \nabla_0 \gamma^x \quad \text{for } \xi = 1, 2, \ldots, 18
\]

(25)

where summation over \( x \) is supposed and where the terms \( d_{\xi} \) include the magnitude of the Burgers vector and relevant slip system directions and products as defined in Eqs. (22) and (23). Eqs. (24) and (25), to be satisfied all over the domain volume \( V_0 \) in the reference state, are reformulated into their integral weak form. Manipulating Eq. (24) gives

\[
\int_{V_0} (\nabla_0 w_u)^T : P^T dV_0 = \int_{A_0} w_u \cdot t_0 dA_0 \quad \text{for all } w_u(x_0)
\]

(26)

with \( A_0 \) the surface enclosing \( V_0; t_0 \), the surface traction and \( w_u(x_0) \), an arbitrary (weighting) vector function depending on the position vector \( x_0 \) in \( V_0 \).

Similarly, Eq. (25) is equivalent to:

\[
\int_{V_0} (w^\xi_\rho \rho_{\text{GND}}^\xi + (\nabla_0 w^\xi_\rho) \cdot d_{\xi} \cdot \gamma^x) dV_0 = \int_{V_0} w^\xi_\rho \rho_{\text{GND}_0} dV_0 + \int_{A_0} w^\xi_\rho \Gamma_0^\xi dA_0 \quad \text{for all } w^\xi_\rho(x_0) \text{ with } \xi = 1, 2, \ldots, 18
\]

(27)

where \( \Gamma_0^\xi \) (with \( \xi = 1, 2, \ldots, 18 \)) represent slip measures along the boundary and \( w^\xi_\rho(x_0) \) are weighting functions depending on the position \( x_0 \) in \( V_0 \). To simplify the elaboration, it is assumed that along external boundaries \( A_0 \) crystallographic slip is obstructed in such a way that it is justified to substitute \( \Gamma_0^\xi = 0 \). This condition reflects e.g. the presence of a hard (oxide) layer at the boundary. To pursue an iterative solution strategy, Eqs. (26) and (27) are rewritten in their weak form:

\[
\int_{V_0} (\nabla_0 w_u)^T : P^* dV_0 = \int_{A_0} w_u \cdot t_0 dA_0 - \int_{V_0} (\nabla_0 w_u)^T : P^{*T} dV_0 \quad \text{for all } w_u(x_0)
\]

(28)

and

\[
\int_{V_0} (w^\xi_\rho \rho_{\text{GND}}^\xi + (\nabla_0 w^\xi_\rho) \cdot d_{\xi} \cdot \gamma^x) dV_0 = - \int_{V_0} (w^\xi_\rho (\rho_{\text{GND}}^\xi - \rho_{\text{GND}_0}) + (\nabla_0 w^\xi_\rho) \cdot d_{\xi} \cdot \gamma^x) dV_0
\]

for all \( w^\xi_\rho(x_0) \) while \( \xi = 1, 2, \ldots, 18 \)

(29)

In these equations the variations (denoted by \( \delta \)) are taken with respect to an estimate indicated by a superscript *. Given suitable estimates for the nodal degrees of freedom (\( u^* \) and \( \rho_{\text{GND}}^\xi \)) at the end of a time increment, the right-hand sides of Eqs. (28) and (29) constitute residuals that have to vanish upon convergence.

The evaluation of the right-hand sides of (28) and (29) is carried out through numerical integration, requiring the kernel to be calculated at the integration points. This implies that it is necessary to compute \( P^* \) and \( \gamma^x \) from the estimates \( u^* \) and \( \rho_{\text{GND}}^\xi \). To compute \( \delta u \) and \( \delta \rho_{\text{GND}}^\xi \) from Eqs. (28) and (29) the variations \( \delta P \) and \( \delta \gamma^x \) in the left-hand sides should be linearly expressed in the variations \( \delta u \) and \( \delta \rho_{\text{GND}}^\xi \). Then, Eqs. (28) and (29) lead to a set of ordinary linear equations.

The calculation of \( P^* \) and \( \gamma^x \) at the integration point level requires the following steps:

1. Starting from an estimate for the incremental slip rates \( \dot{\gamma}^x \), determine the plastic part of the deformation gradient tensor \( F_p^* \) by integrating equation (3) to yield \( F_p^* = (1 + \Delta t \lambda_p) \cdot F_p \) where \( F_p \) denotes the previous deformation gradient and \( \Delta t \) is the current time step.
2. With \( F_p^* \) and the current deformation gradient \( F^* \) obtained from the FEM displacement field, determine the associated elastic deformation gradient tensor \( F_e^* \) with Eq. (1). Subsequently compute the second Piola–Kirchhoff stress tensor \( S^* \) using Eq. (4). Use this result to determine the resolved shear stresses \( \tau^{xz} \) on the slip systems \( z \) by applying Eq. (6).

3. Determine the first Piola–Kirchhoff stress tensor \( P^* \) according to:

\[
P^* = \tau^* \cdot F^{*(-T)} = F_e^* \cdot S^* \cdot F_e^{*(-T)} = F_e^* \cdot S^* \cdot F_e^{*(-T)}
\]

where it is recalled that the second Piola–Kirchhoff stress tensor \( S^* \) was related to the intermediate configuration while the first Piola–Kirchhoff stress tensor \( P^* \) was defined with respect to the undeformed reference state.

4. Determine the dislocation induced stress tensors from the GND density fields defined by the nodal values \( p_G^* \) using Eqs. (15) and (16) and then calculate the back stresses \( \tau_b^{xz} \) on the slip systems with Eq. (19). From \( \tau^{xz} \) and \( \tau_b^{xz} \) determine the effective shear stresses with Eq. (8).

5. Evaluate the right-hand side of the slip law equation (7). The results will deviate from the current slip rate estimates \( \dot{\gamma}^{xz} \). The differences give an indication how the estimates should be adapted and, as long as convergence is not yet reached, the next iteration step (restarting the procedure from step 1) can be executed.

When \( P^* \) and \( \dot{\gamma}^{xz} \) (for \( z = 1, 2, \ldots, 12 \)) have been computed, the right-hand sides of Eqs. (28) and (29) can be determined. Based on these residuals, global iterative corrections \( \delta u \) and \( \delta p_G^* \) have to be calculated. This iterative process is repeated until the residuals are sufficiently small, i.e. until convergence has been obtained. Further details of the FEM implementation can be found in Evers et al. (2004b).

5. Application to constrained simple-shear

Simple shearing of a constrained strip has been examined by Shu et al. (2001), Evers et al. (2004a), Bitten-court et al. (2003) and Fredriksson and Gudmundson (2005) and leads to the development of deformation gradients resulting in boundary layers with vanishing plastic deformation. Since these deformation gradients form at the onset of plastic deformation, it is an ideal configuration to examine the difference in the two back stress formulations proposed in Section 2.2. The previously cited gradient crystal plasticity and dislocation dynamics simulations employed models with a restricted number of slip systems, which neglect out-of-plane slip. In the following therefore, two slip system configurations are examined: double-planar and octahedral slip, to examine the influence of the number of available slip systems on the deformation profile and in particular the difference in the latent hardening behaviour.

For the double-planar slip case, the two slip systems are assumed to lie on one of the \{111\} close-packed slip planes of an FCC crystal, with slip directions of [101] and \( \frac{1}{2} [112] \), such that the slip directions lie at 60° from the horizontal axis as drawn in Fig. 3. In the case of octahedral slip, all the 12 close-packed slip systems listed in Table 1 are considered with their crystallographic orientations shown in Fig. 4.

A sample with a constant height \( H \) of 0.22 mm is considered, which has been discretized with a column of 30 four-noded plane-strain (in \( x_3 \) direction) elements. An infinite sample width (in \( x_1 \) direction) is represented by applying periodic boundary conditions, which tie the nodal degrees of freedom along the left and right

![Fig. 3. Geometry and boundary conditions for the double-planar simple shear configuration.](image-url)
boundaries. Consequently, gradients in both the $x_1$ and $x_3$ directions vanish, such that slip gradients and $\rho_{\text{GND}}$ can only develop in the $x_2$ direction. The assumption that $I_0^c = 0$ along the external surfaces in Eq. (27) enforces that surface-normal crystallographic slip is prohibited, representative of a slip obstructing grain boundary, see Shu et al. (2001).

Material parameters used in the simulations are listed in Table 2 and are identical to those employed in an earlier investigation of copper single crystals by Evers et al. (2004b). For the double-planar slip configuration, only self-hardening (SH) and coplanar hardening (CP) are employed, while for the octahedral slip configuration all six interaction coefficients are specified. Along the lower surface the applied boundary conditions are $u_1 = u_2 = u_3 = 0$, $I_0^c = 0$ while along the upper surface $u_1 = \dot{\gamma} \Delta t H, u_2 = u_3 = 0$, and $I_0^c = 0$.

5.1. Results

A constant shear rate of $|\dot{\gamma}| = 1 \times 10^{-3}$ s$^{-1}$ is applied to a maximum of 2% shear, with two load reversals at 1% and 2%, to assess the influence of the two different back stress formulations during reversed plasticity. To examine the importance of the material length scale $R$ in Eqs. (15) and (16), a range of values between $0 < R \leq 25$ µm are taken for both slip system configurations.

Shear stress versus shear displacement curves are reported in Fig. 5a and b for the double-planar and octahedral slip cases, respectively while the influence of the material length scale $R$ is examined separately in Fig. 6. For the non-zero internal length scale cases (i.e. $R \neq 0$), the response exhibits the classical Bauschinger effect where the absolute value of the reversed yield point occurs at stress levels lower than the unloading point. This is consistent with the increased kinematic hardening arising from the internal stress contribution and is seen to be dependent on the back stress formulation, the number of available slip systems, and the magnitude of the material length scale. When slip is restricted to the double-planar configuration, the predominance of the Bauschinger effect is exaggerated, and after unloading at 2% shear plastic unloading occurs for the full internal stress formulation, which in this case is due to the relatively high value of $R$. Although not observed in polycrystalline materials, plastic behaviour during unloading has been observed experimentally during nano-indentation of silicon nanoparticles and was attributed to the enormous back stresses that develop when dislocations are only a few nanometers apart, see Gerberich et al. (2005).

While the two slip system configurations and different internal stress formulations generate different response curves, the deformation profiles are nearly indistinguishable when $R \neq 0$ as plotted in Fig. 7 after 1% and 2% shear. Thus the kinematics of the crystallographic slip is largely independent of the slip system configuration and the adopted back stress formulation. While five independent slip systems are typically required to achieve an arbitrary (isochoric) deformation, the orientations of the double-planar slip systems with respect to the shearing direction are suitable to correctly capture the slip kinematics, however as will be pointed out later, with limited latent hardening.
Beyond the onset of plastic deformation, a heterogeneous deformation profile develops in response to the imposed boundary condition of $I_0 = 0$ along the upper and lower surfaces as plotted in Fig. 7 after 1% and 2% shear. This heterogeneous deformation profile continues to develop with increased plastic deformation and is in contrast to the near-homogeneous profile predicted when the internal stresses are neglected (i.e. if $R = 0$).
The material length scale $R$ serves to amplify the effect of the back stress contribution. Setting $R = 0$, the back stress contribution is omitted from the constitutive response, and the GNDs only contribute to the slip system resistance ($\sigma^s$), with near isotropic hardening rates evident in Fig. 5 and no Bauschinger effect during reversed loading. Thus setting $R = 0$ for each slip system configuration provides a reference hardening rate with which the results including the internal stress formulations can be compared. With an increasing back stress contribution the Bauschinger effect becomes more pronounced as the extent of kinematic hardening.

Fig. 7. Deformed profile of an initially vertical bar showing the correspondence between the two slip system configurations, and internal stress formulations at deformations corresponding to $\gamma = 0.01$ and $\gamma = 0.02$. The gray band represents the indistinguishable deformation profiles obtained for the double-planar and octahedral slip configurations and the two internal stress formulations. The deviation from linearity originates from the imposed boundary condition $u_0 = 0$ along the upper and lower surfaces.

Fig. 8. Vertical $\gamma^s$ distributions for $\gamma = 0.02$. In (b), the $z$ labels refer to pairs of nearly indistinguishable slip rates that form on colinear slip systems, which develop independently of the internal stress formulation. (a) Double-planar slip ($\alpha = 1$) and (b) octahedral slip.
increases. In order to examine the origins of this kinematic hardening and differences between the two slip system configurations, the slip rates, GND density and back stress distributions are examined after an applied shear of $\gamma = 0.02$ and $R = 25 \mu m$.

Fig. 8a and b presents the slip rate distributions in the vertical $x_2$ direction for the double-planar and octahedral slip configurations. Approaching the upper and lower boundaries, the slip rates tend to zero as a consequence of the imposed boundary condition $C_n = 0$ which results in a size dependent boundary layer. Considering the case of octahedral slip plotted in Fig. 8b, pairs of slip rates develop in response to the lattice symmetry and applied loading conditions, with a net crystallographic shape change resulting from the contribution of slip systems with opposite slip directions. No crystallographic slip develops along the $\{001\}$ plane as a consequence of the imposed plane-strain and periodic boundary conditions. In agreement with the indistinguishable deformation profiles plotted in Fig. 7, the slip rates for the two internal stress formulations are similar, differing only slightly at the mid section.

Approaching the upper and lower surfaces, where the crystallographic slip vanishes, the GNDs develop in order to enable a gradient in the slip rates according to Eqs. (22) and (23) as plotted in Fig. 9. Along the $\{100\}$ planes edge dislocations are formed while screw dislocations accumulate on the $\{010\}$ planes. All of the GNDs accommodate slip gradients in the $x_2$ direction, since the periodic and plane strain boundary condition preclude plastic deformation gradients in the other directions. For both the double planar and octahedral slip configurations, the influence of the back stresses on the GND distribution are clearly seen in Fig. 9. When the influence of the back stress is neglected (i.e. setting $R = 0$) the GNDs form a very localized boundary layer, while increasing the magnitude of the back stresses results in a more diffuse GND distribution, concluding that the thickness of the boundary layer is related to the magnitude of the material length scale.
While the slip system kinematics are similar for the two internal stress formulations, the resolved back stress ($\tau_{ab}$) distributions are significantly different as plotted in Fig. 10. As defined in (15) and (16), the back stresses develop from the gradients of the GND densities plotted in Fig. 9 with increased back stresses when approaching the upper and lower surfaces. The origin of the Bauschinger effect observed in Fig. 5 during unloading can be inferred from Fig. 10 since during unloading the sign of $\tau^a$ will change while $\tau_{ab}$ will remain constant and hence the magnitude of the effective stress ($\tau_{eff}$) will change. With increasing back stresses the Bauschinger effect becomes more dominant as observed for the double-planar slip configuration as plotted in Fig. 5.

The difference in the hardening rates observed in Fig. 5 for the two internal stress formulations can be attributed to the differences in the resolved back stress ($\tau_{ab}$) as plotted in Fig. 10. Independent of the slip configuration and internal stress formulation, the crystallographic slip rates plotted in Fig. 8 are similar. This implies that the ratio $(\tau^a - \tau_{ab})/s^a$ in Eq. (7) is nearly independent of the internal stress formulation. Since the vertical GND and SSD distributions are similar, the slip resistance ($s^a$) is also independent of the selected internal stress formulation, and therefore to satisfy the slip rate equality, $\tau^a$ must be different to overcome $s^a$ as plotted in Fig. 10 for the two slip configurations.

6. Discussion

6.1. Latent hardening

The hardening rates observed in Fig. 5 for the two different slip system configurations and different back stress formulations appear to be contradictory. For example the full internal stress formulation of the
double-planar configuration has a greater hardening rate than the self-internal formulation, while for the octahedral slip configuration, the self-internal formulation gives the greater hardening rate. This dichotomy originates from the superposition of the dislocation induced stress fields. This is illustrated for the octahedral slip system case by artificially enforcing a constant dislocation gradient of ±10 μm⁻³ for each of the non-zero GND gradients (i.e. \( n = 3, 6, 9, \) and 12 for the edge dislocations and \( n = 14 \) and 17 for the screw components) that developed during simple shear as plotted in Fig. 9b. The resolved back stresses associated with these gradients are obtained from Eqs. (15), (16 and (19) and are plotted in Fig. 11. The column heights in Fig. 11 reflect the total resolved back stress accumulated over all of the slip systems where the contributions emerging from edge GNDs and screw GNDs are indicated by the different patterns.

For the full internal stress formulation, the screw dislocation gradients do not contribute to the net resolved back stress since opposing back stresses develop on each slip system when \( n = 14 \) and \( n = 17 \). These pairs of equivalent screw GND gradients develop as a result of the crystal symmetry for the present case of simple shear, and therefore, the self-internal formulation develops a greater net resolved back stresses on each slip system than the full internal stress formulation.

The dichotomy of the hardening rates between the two slip system configurations plotted in Fig. 5 results from the difference in latent kinematic hardening and in particular the omission of the screw dislocation gradients in the case of double-planar slip. The difference in the kinematic hardening can be examined by first considering only the self-hardening characteristics of the two internal stress formulations. For an edge dislocation gradient, the back stresses on the slip system associated with this dislocation are found to be independent of the internal stress formulation, and therefore, the differences in the kinematic hardening arise solely from the latency of the remaining slip systems. The effect of this increased latent hardening for the full internal stress formulation is evident in Fig. 11 where the combined back stresses arising from four edge dislocations are greater than that obtained from the self-internal stress formulation. The significance of this latent hardening difference appears in Fig. 5a as an increased macroscopic hardening rate for the full internal stress formulation. However, when the both edge and screw dislocations are included i.e. the octahedral slip case, the back stresses associated with the screw dislocations override the relatively small increase in latent hardening, and the self-internal stress formulation results in the larger macroscopic hardening rates as seen in Fig. 5b.

The decision to include the dislocation induced stress components in directions other than along the slip plane, introduces the tensorial nature of the stress state on the material. This arrangement describes more completely the dislocation induced stress field, and hence is a more sensible description of the dislocation induced stress field than the termed self-internal stress formulation, which only accounts for the dislocation induced stresses acting along the slip system.

6.2. Material length scale

Strain gradient material models are capable of capturing material size dependence by including the GNDs required to satisfy lattice compatibilities. As plotted in Fig. 9, these GNDs develop a boundary layer within
which crystallographic slip is impeded by both the increased slip system resistance and the presence of a back stress associated with the long range GND interactions. The extent of this boundary layer is dependent upon the magnitude of the material length scale $R$ and as shown in Fig. 6 has a pronounced effect on the global behaviour. In the present formulation, the intrinsic material length scale $R$ in Eqs. (15) and (16) acts as a gradient multiplier and is the radius within which individual dislocations contribute to the internal stress field. Although derived differently, the form of the self-internal stress formulation parallels that of Yefimov et al. (2004) and Yefimov and Van der Giessen (2005):

$$
\tau_s(x_0) = \frac{G b}{2 \pi (1 - v) \rho(x_0)} \cdot D \frac{\partial \rho_{\text{GND}}}{\partial x_0}
$$

except from their use of $1/\rho(x_0)$ and the omission of any latent hardening effects as dealt with in this paper. The term $\rho(x_0)$ relates to the total dislocation density including both the contribution of SSDs and GNDs and is comparable to using a variable length scale in the present formulation, if the substitution $R^2 = 1/\rho$ is made in Eqs. (15) and (16). In this case the length scale would take the smallest possible value representing only nearest neighbor dislocation interactions.

The use of a variable length scale in gradient plasticity has been shown by Voyiadjis and Abu Al-Rub (2005) to yield better agreement between experimentally acquired micro-bending (Stölken and Evans, 1998), and micro-torsion (Fleck et al., 1994) results of pure metallic films and wires, respectively. However, as the dislocation induced internal stress arises from the interaction between dislocations, considering only nearest neighbor interactions surely underestimates the back stress contribution as considered in Eq. (31) since in regions with a high dislocation density, and hence a correspondingly small dislocation spacing, the internal stress contribution would be negligible. In order to compare the magnitude of this interaction region with one of the static length scales considered in this paper, the dislocation spacing determined as $(\rho_{\text{GND}})^{-1/2}$ is plotted in Fig. 12 at the lower boundary. As expected, the interaction region associated with the nearest neighbor interactions is initially large, but rapidly approaches a value of approximately $R = 1 \, \mu m$ with increased shear deformation. If the material length scale was set to such a small value, the results would approach those of $R = 0$ which exhibit no Bauschinger effect, limited boundary layer thickness with a consequently reduced size dependency.

Therefore, it is concluded that an interaction region larger than nearest neighbor dislocation spacing is required in order to capture these effects. Nevertheless, a variable length scale is expected to be more realistic for which a second-order estimate based on for example, the second gradient of the dislocation density could be used.

Fig. 12. Nearest neighbor interaction distance determined as the dislocation spacing $(\rho_{\text{GND}})^{-1/2}$ for both screw and edge GNDs as a function of applied shear. Plotted alongside the inter-dislocation spacing is the static material length scale $R$ used in the calculation of the internal stress field.
7. Conclusion

An internal stress formulation has been proposed in which the full tensorial nature of the dislocation induced stresses is taken into account. The formulation differs from previously defined procedures to determine internal stresses, i.e. (Evers et al., 2004a,b) since it includes not only the stress components acting in the slip system direction due to the dislocations on that slip system, but also the contribution of all other slip system dislocations, and hence leads to a more realistic representation of the dislocation induced internal stresses. For the case of simple shear of a single FCC crystal material with either double-planar or octahedral slip, the following conclusions can be drawn.

- While double-planar slip configurations are adequate to represent correctly the deformation kinematics of simple shear, it fails to adequately capture slip system interactions resulting in different latent hardening behaviour than obtained using all 12 octahedral FCC slip systems. Furthermore, omitting the development of screw dislocations, significantly alters the back stress contribution, and consequently the global hardening behaviour.
- The full internal stress formulation has an increased latent hardening compared to the self-internal stress formulation for both edge and screw dislocation gradients. However, for the case of simple shearing of a cube oriented single crystal, crystal symmetry and counteracting stress states from equal dislocation gradients, neglect the screw dislocation contributions.
- The two dislocation induced internal stress formulations have a pronounced effect on the global behaviour, in particular the observed Bauschinger effect resulting from the different back stresses on the active slip system. While the choice of internal stress formulations influences the applied flow stress, the kinematics of the deformation are hardly affected.
- In order to adequately capture size dependent behaviour and latent kinematic hardening associated with the Bauschinger effect, the material length scale $R$, should be larger than the interaction region associated with nearest neighbor dislocations.

References


