Crystal plasticity model with enhanced hardening by geometrically necessary dislocation accumulation

L.P. Evers\textsuperscript{a,b,*}, D.M. Parks\textsuperscript{c}, W.A.M. Brekelmans\textsuperscript{b}, M.G.D. Geers\textsuperscript{b}

\textsuperscript{a}Netherlands Institute for Metals Research (NIMR), The Netherlands
\textsuperscript{b}Section of Materials Technology, Department of Mechanical Engineering, Eindhoven University of Technology, PO Box 513, 5600 MB Eindhoven, The Netherlands
\textsuperscript{c}Massachusetts Institute of Technology, Department of Mechanical Engineering, Cambridge, MA 02139, USA

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Abstract

A strain gradient dependent crystal plasticity approach is used to model the constitutive behaviour of polycrystal FCC metals under large plastic deformation. Material points are considered as aggregates of grains, subdivided into several fictitious grain fractions: a single crystal volume element stands for the grain interior whereas grain boundaries are represented by bi-crystal volume elements, each having the crystallographic lattice orientations of its adjacent crystals. A relaxed Taylor-like interaction law is used for the transition from the local to the global scale. It is relaxed with respect to the bi-crystals, providing compatibility and stress equilibrium at their internal interface. During loading, the bi-crystal boundaries deform dissimilar to the associated grain interior. Arising from this heterogeneity, a geometrically necessary dislocation (GND) density can be computed, which is required to restore compatibility of the crystallographic lattice. This effect provides a physically based method to account for the additional hardening as introduced by the GNDs, the magnitude of which is related to the grain size. Hence, a scale-dependent response is obtained, for which the numerical simulations predict a mechanical behaviour corresponding to the Hall–Petch effect. Compared to a full-scale finite element model reported in the literature, the present polycrystalline crystal plasticity model is of equal quality.
yet much more efficient from a computational point of view for simulating uniaxial tension experiments with various grain sizes. © 2002 Elsevier Science Ltd. All rights reserved.

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1. Introduction

It is well known that the grain size has a dominant influence on the mechanical behaviour of polycrystalline metals and alloys. This dependence is not taken into account by approaches as proposed by Taylor (1938). In the past, many applications of Taylor-type models (e.g. Asaro and Needleman, 1985) have been used for describing the behaviour and texture evolution of FCC polycrystals during large plastic deformation. Additionally, Bronkhorst et al. (1992) showed that the Taylor model provides an acceptable description of the behaviour of single-phase FCC polycrystals under pure slip deformation. However, in this model, a homogeneous deformation field across grain boundaries and within grains is assumed, neglecting differences in structure from grain to grain and within grains. Nevertheless, the continuity across grain boundaries could also be upheld when the deformation inside a grain was inhomogeneous, in other words if the crystal boundary region deformed dissimilar from the crystal interior (Kochendörfer, 1941). This hypothesis initiated the suggestion by Nabarro (1950) and Boas (1950) that the flow stress might depend on the grain size. In fact, it is this hypothesis which constitutes the basis of the micromechanical model in this work.

Hall (1951) and Petch (1953) first examined the grain size dependence and found an empirical relationship between the crystal size $d$ and the yield stress, which was extended by Armstrong et al. (1962) to include the entire flow stress region $\sigma(\varepsilon)$ by expressing the parameters $\sigma_0$ and $k$ to be dependent on the strain level $\varepsilon$ in a relation known as the (extended) “Hall–Petch relation”

$$\sigma(\varepsilon) = \sigma_0(\varepsilon) + k(\varepsilon)d^{-n}.$$  

In the literature, values for the exponent $n$ in the range of 0.3 to 1 show the best resemblance with experimental findings, whereas $n = \frac{1}{2}$ is the most reported value. The Hall–Petch slope $k$ characterizes the transfer of slip through the grain boundaries. For a more detailed discussion of the flow stress dependence on the grain size, see Hansen (1982) and Narutani and Takamura (1991), and references therein.

Three different models can be distinguished (Gavriljuk et al., 1999) which explain the strengthening effect of smaller grains. First, the “dislocation pile-up models” state that the propagation of plastic deformation is obstructed at the crystal boundaries by stress concentrations as caused by the pile-up of dislocations, which in their turn activate dislocation sources in neighbouring grains (Hall, 1951; Petch, 1953; Cottrell, 1958; Nakanishi and Suzuki, 1974; Suzuki and Nakanishi, 1975). These models focus on the restricted dislocation movement across grain boundaries, which affect the flow stress in Eq. (1) through $d^{-1/2}$. The main objection against this explanation is that in metals
with a BCC crystal structure, no pile-ups are observed while the Hall–Petch relation is nevertheless retrieved. Second, the “dislocation interaction models” (or “work hardening models”) (Ashby, 1970; Hirth, 1972; Conrad, 1963; Dai and Parks, 1997; Dai, 1997; Arsenlis and Parks, 2000) emphasize the increased concentration of dislocations by affirming that the dislocation density accumulated in a grain at a certain strain is higher once the grain size decreases, which is inherent to the increased inhomogeneous deformation (i.e., strain gradients) within the grain and the accompanying decreasing mean free path of the dislocations. These models predict values for the exponent \( n \) in the total range mentioned. Finally, the “grain boundary source model” (Li and Chou, 1970) emphasizes the capacity of grain boundaries to emit dislocations under loading, which does not require a stress concentration created by a pile-up. However, up till now, no clear experimental evidence has been able to support the exclusive validity of any of these models.

The dislocation interaction approach has been extended by Ashby (1970). Hardening, i.e., resistance to dislocation motion, is caused by secondary dislocations piercing the slip planes, which multiply during plastic deformation and increase the slip resistance. In that work, a distinction is made between statistically stored dislocations (SSDs), accumulating during a uniform deformation, and geometrically necessary dislocations (GNDs), which are required to preserve lattice compatibility in the case of unevenly distributed plastic slip (non-uniform plastic deformation, such as in the presence of lattice curvature). As suggested by Kocks (1970) and sustained by Thompson et al. (1973), geometrically necessary dislocations are largely concentrated in the grain boundary regions where the lattice mismatch is most pronounced. Supporting this, Kazmi and Murr (1979) highlighted the formation of high dislocation densities in the vicinity of grain boundaries by means of transmission electron microscopy.

Several strain gradient models have been developed in order to numerically capture scale size effects (e.g. Aifantis, 1987; Fleck et al., 1994; Fleck and Hutchinson, 1997; Gao et al., 1999; Huang et al., 2000; Shu and Fleck, 1999; Dai and Parks, 1997; Dai, 1997; Shi et al., 2000). Such approaches incorporate a length scale in the analytical plasticity formulation, thereby enabling the prediction of e.g. particle size effects and indenter size effects. The underlying physics is sometimes related to the SSD and GND generation (Gao et al., 1999). However, limitations are met with respect to two-dimensional idealizations of double slip and the consideration of global strain gradients instead of intragranular strain gradients, respectively absent and present in a macroscopically uniform deformation mode. In the present work, a scale-dependent theory of plastic strain gradient induced production of GNDs is elaborated, based on the work of Arsenlis and Parks (2000), in the context of which intragranular strain gradients can be accounted for.

In the model to be developed, each crystallographic orientation in a material point is associated with a grain. This grain is considered to have a material volume fraction assigned to its core, whereas the remaining volume fraction is covered by its boundary volume elements. The heterogeneous deformation within a crystal, typically occurring between the crystal core and the grain boundaries, initiates the generation (either through nucleation or dislocation motion) of geometrically necessary dislocations to maintain lattice compatibility. These GNDs cause in their turn the slip resistance near
the grain boundaries to increase, as experimentally shown by Worthington and Smith (1964). This extra hardening is merely assigned to the boundary volume elements. Despite the fact that in this way the dislocations are practically “stored” (piled-up) near the boundaries, this model mainly lies in the range of the “dislocation interaction models”.

Note that the grain diameter is a model parameter used to determine the measure of inhomogeneity. No explicit flow stress relation depending on the grain diameter (e.g. according to Eq. (1)) is included in the model (cf. Thompson et al., 1973). Furthermore, the approach of Meyers and Ashworth (1982) and its extension by Fu et al. (2001) also relied on a subdivision of grains into an interior section and a surrounding grain boundary region. The grain subdivision is based on the increased hardening rate near the grain boundaries (experimentally verified by Gray III et al., 1999), an observation which is expected to be the result of the compatibility requirements near those boundaries. Subsequently, Fu et al. took this effect into account through different evolution coefficients of the dislocation densities in the core and near the boundaries. Moreover, again, a flow stress relation was required in which the diameter dependence entered explicitly (in this case through geometrical considerations). In the approach presented in this contribution, on the other hand, the constitutive material parameters are kept equal in the core and in the grain boundary layer (the bi-crystals) and the increased hardening term in the grain boundary section only arises to the extent in which it is physically motivated, i.e., only when there is -and in proportion to- a deformation incompatibility.

The constitutive crystal plasticity framework is based on the work of Bronkhorst et al. (1992) and Kalidindi et al. (1992). However, in such local continuum constitutive models, no explicit attention is paid to the presence of GNDs and no absolute length scale enters the formulations. Therefore, they implicitly assume that the accumulation of SSDs is the only driving force behind the work hardening, which is related to the history of the crystallographic plastic shear strains.

As mentioned before, Taylor-type models assume deformation uniformity within grains and across grain boundaries, violating the stress equilibrium condition at the interfaces. Alternatively, their counterpart, the Sachs-type models, assume the stress to be uniform, neglecting kinematical compatibility. In the case of intermediate models, the consideration of intergranular processes accounts for both the consistency conditions of grain boundary compatibility and traction equilibrium to be satisfied. This makes intermediate models, such as for example the self-consistent models, more rational. Self-consistent approaches, however, involve severe assumptions in order to simplify the formulations and to reduce the computation time (Molinari et al., 1997). The present contribution contains an alternative intermediate model, which is based on a relaxed form of the Taylor assumption. Unlike the classical assumption, in this work, one grain consists of several fractions (i.e., representative volume elements). The crystal interior is modelled by one single crystal volume element, whereas several bi-crystal volume elements represent the grain boundaries. The Taylor assumption is now applied to the deformation of the single crystal core and the average deformation of each bi-crystal component. Additionally, at the interface within the bi-crystals, the consistency conditions of deformation compatibility and stress equilibrium are imposed.
In this way, the above mentioned intragranular deformation heterogeneity arises, which is here concentrated between the core and the bi-crystals of each grain.

The approach of using a bi-crystal in combination with Taylor’s assumption originates from the work of Ahzi et al. (1990), where a two-phase composite inclusion was used as a representative volume element of crystalline lamella and its associated amorphous layer in two-phase semi-crystalline polymers. The extension of this approach for the modelling of grain boundaries of FCC metals by choosing the composite inclusion to be a bi-crystal, having the lattice orientations of the two neighbouring crystals, was first performed by Lee et al. (1999). However, in their contribution, only the crystal interfaces are taken into account, leaving the crystal interiors unconsidered. Furthermore, Delannay et al. (1999) refer to a similar approach of bi-crystal modelling by means of the “Lamel model”. An empirical examination of the presence of GNDs near the grain boundaries of an aluminium bi-crystal, measured through lattice curvatures, can be found in Sun et al. (2000).

First, the general crystal plasticity constitutive framework and its time integration are outlined in Section 2. Next, in Section 3, the subdivision of a grain into a core and several bi-crystal boundaries is discussed, along with the complementary time integration procedure. In Section 4, the deformation incompatibility between the core and the boundaries is considered, which induces the production and accumulation of GNDs. This extra dislocation density obstructs the dislocation motion and hence introduces enhanced hardening. Further, in Section 5, the computational results of uniaxial tensile tests are compared to experimental results obtained by Hansen (1979) and to numerical results obtained by Arsenlis and Parks (2000), both describing Hall–Petch-like behaviour. Arsenlis and Parks considered a collection of grains, where each grain is discretized in finite elements. Hereby, the strain gradients arise from the deformation heterogeneity between the different finite elements, i.e., between elements near the core and elements near the boundary. From those strain gradients, the enhanced hardening arises and the corresponding slip resistance can be determined after consideration of the GND densities. Finally, concluding remarks are made in Section 6.

2. Crystal plasticity framework

2.1. Kinematics

The kinematics commonly used in the field of crystal plasticity may be traced back to the works of Lee (1969), Rice (1971), Hill and Rice (1972), and Asaro and Rice (1977). The basic feature is the distinction between two physical mechanisms, represented by the multiplicative decomposition of the deformation gradient tensor

\[ F = F_e \cdot F_p. \]  

(2)

The elastic part \( F_e \) comprises the small lattice deformation and possibly large rigid body rotation. The plastic part \( F_p \) corresponds to the isoclinic and stress-free intermediate configuration, in which the crystallographic lattice is unaltered and unrotated with respect to the reference configuration (Mandel, 1974), as illustrated in Fig. 1. It is
assumed that this part results solely from continuous plastic shearing (dislocation motion) on well-defined slip systems. For FCC metals, 12 favourable (octahedral) systems can be characterized by the Miller indices \( \{111\}, \langle 110 \rangle \), where each system \( \alpha (\alpha = 1, 2, \ldots, 12) \) is represented in the reference configuration by the two time-independent orthonormal vectors \( m_0^\alpha \) and \( n_0^\alpha \), the slip direction and slip plane normal, respectively. Now, the evolution of the plastic deformation can by definition be expressed as the superposition of all crystallographic slip rates \( \dot{\gamma}^\alpha \) (Rice, 1971)

\[
\dot{F}_p = L_p \cdot F_p, \quad L_p = \sum_{\alpha} \dot{\gamma}^\alpha P_0^\alpha, \quad P_0^\alpha \equiv m_0^\alpha n_0^\alpha,
\]

where \( L_p \) is the plastic velocity gradient tensor and \( P_0^\alpha \) is known as the non-symmetric Schmid tensor.

### 2.2. Constitutive model

The second Piola–Kirchhoff stress measure defined with respect to the relaxed configuration

\[
\tau \equiv \det(F_e)F_e^{-1} \cdot \sigma \cdot F_e^{-T},
\]

with \( \sigma \) the Cauchy stress tensor, is taken to be related to its work conjugated elastic Green strain measure \( E_e \) through

\[
\tau = 4C : E_e, \quad E_e \equiv \frac{1}{2}(C_e - I), \quad C_e \equiv F_e^T \cdot F_e,
\]

where \( C_e \) is the elastic right Cauchy–Green tensor and \( I \) is the second-order unit tensor. The fourth-order isotropic elasticity tensor \( 4C \) is defined by Young’s modulus \( E \) and Poisson’s ratio \( v \)

\[
4C = \frac{\nu E}{(1 + \nu)(1 - 2\nu)} \left( I^I + \frac{1 - 2\nu}{\nu} 4I \right),
\]

where \( 4I \) is the symmetric fourth-order unit tensor.
To arrive at an elasto-viscoplastic material model, the plastic shearing rate $\dot{\gamma}^x$ is expressed as a power law function of the slip system resolved shear stress $\tau^x$ and deformation resistance $s^x$ according to the flow rule (Hutchinson, 1976; Peirce et al. 1982)

$$\dot{\gamma}^x = \dot{\gamma}_0 \left\{ \frac{\tau^x}{s^x} \right\}^{1/m} \text{sign}(\tau^x),$$

(7)

where $\dot{\gamma}_0$ and $m$ are material parameters representing the reference plastic strain rate and the rate sensitivity exponent, respectively. The “Schmid stress” $\tau^x$ is defined such that $\sum_{\beta} |\tau^x \dot{\gamma}^x|$ is precisely the rate of plastic work per unit volume in the relaxed configuration (Asaro and Rice, 1977; Bronkhorst et al., 1992)

$$\tau^x \equiv C_e \cdot \tau : P^x_0.$$  

(8)

For metallic materials, the elastic strains are usually negligibly small. For this situation, the resolved shear stress $\tau^x$ in Eq. (8) may be approximated by

$$\tau^x \approx \tau : P^x_0.$$  

(9)

The slip resistance $s^x$ in Eq. (7) is taken to evolve according to the expression (Asaro, 1983; Kalidindi et al., 1992)

$$s^x = \sum_{\beta} h^{x\beta} |\dot{\gamma}^{\beta}|, \quad s^x(t = 0) = \tau_0,$$

(10)

where $\tau_0$ is the initial slip resistance, which is considered to be equal for each slip system. The hardening moduli $h^{x\beta}$ give the rate of strain hardening on slip system $x$ due to slip on slip system $\beta$. For now, this occurrence of self and latent hardening is phenomenologically described by

$$h^{x\beta} = q^{x\beta} h^{\beta} \quad \text{(no sum on $\beta$)},$$

(11)

where $q^{x\beta}$ equals unity for coplanar slip systems and the scalar value $q$ for non-coplanar systems. This choice has been motivated by experimental observations performed by Kocks (1970). Finally, the following specific form for the single-slip hardening rate, $h^{\beta}$ in Eq. (11) is adopted, which was originally motivated by the work of Brown et al. (1989)

$$h^{\beta} = h_0 \left( 1 - \frac{s_\beta}{s_\infty} \right)^a,$$

(12)

with the slip system hardening parameters $h_0$, $a$ and $s_\infty$.

### 2.3. Time integration

For each single or bi-crystal volume element of each grain, each having a unique lattice orientation(s), the constitutive response as well as the history dependent variables differ from those of other volume elements with a different orientation, undergoing the same deformation. Therefore, the proposed computational procedure is performed per volume element. First, in this section, the single crystal elements are considered. Next,
in Section 3.2, the complementary time integration procedure for bi-crystal components is given.

Such as typical in implicit finite element codes, for each time increment, an estimated displacement field is used to calculate the stress and to update the state variables in each integration point. This process is repeated for a number of iterations until equilibrium of the global forces is realized for the particular time increment. Consequently, at each new time step ($t_{n+1} = t_n + \Delta t$, in the remainder of this paper, associated variables are denoted with the subscript $n+1$), the plastic deformation and the slip restrictions at the previous time ($t_n$, variables with subscript $n$) are known state variables. Furthermore, the time-independent material parameters and slip system orientations of the grain under consideration are known.

The implicit integration procedure (Eqs. (13)–(21)) is based on the contributions of Bronkhorst et al. (1992) and Kalidindi et al. (1992) and starts with the time integration of Eq. (3)

$$F_{p_{n+1}} = \exp(\Delta t L_{p_{n+1}}) \cdot F_{p_n},$$

which can be approximated by

$$F_{p_{n+1}} \approx (I + \Delta t L_{p_{n+1}}) \cdot F_{p_n}.$$  

(14)

Correspondingly, the first-order estimation of the inverse of $F_{p_{n+1}}$ can be written as

$$F^{-1}_{p_{n+1}} \approx F^{-1}_{p_n} \cdot (I - \Delta t L_{p_{n+1}}).$$

(15)

To compute the stress at the end of the time step, $F_{e_{n+1}}$, determined by

$$F_{e_{n+1}} = F_{n+1} \cdot F^{-1}_{p_{n+1}},$$

(16)

is substituted into Eq. (5), which after employing Eq. (15) leads to

$$\tau_{n+1} = 4C : \left\{ \frac{1}{2} (A - I) - \frac{1}{2} \Delta t (\dot{A} \cdot L_{p_{n+1}} + L^T_{p_{n+1}} \cdot \dot{A}) \right\},$$

(17)

with

$$A \equiv F_{p_n}^{-T} \cdot F_{n+1}^T \cdot F_{n+1} \cdot F_{p_n}^{-1}.$$  

(18)

When the plastic velocity gradient tensor is written in the crystallographic form of Eq. (3), Eq. (17) ends up like

$$\tau_{n+1} = \tau^{tr} - \sum_x \Delta \tau^{x}_{n+1} (\tau_{n+1}, s^x_{n+1}) B^x$$

(19)

with the trial stress (elastic prediction)

$$\tau^{tr} \equiv 4C : \left\{ \frac{1}{2} (A - I) \right\}$$

(20)

and

$$B^x \equiv 4C : \left\{ \frac{1}{2} (A \cdot P^x_0 + P^x_0 \cdot A) \right\}.$$  

(21)

Using this approach, the introduced variables ($A$, $\tau^{tr}$ and $B^x$) are known at time $t_{n+1}$, leaving only the stress $\tau_{n+1}$, slip rates $\dot{s}^x_{n+1}$ and slip resistances $s^x_{n+1}$ to be computed.
The slip rates are computed using Eq. (7) and substituting the implicit time integration of Eq. (10) into this equation leads to

\[
\dot{\gamma}_n^{x} = \gamma_0 \left\{ \frac{\tau_n^{x} |r_{n+1}|}{\tau_n + \Delta t \sum_{\beta} h_{\tau_{\beta}} |\dot{\gamma}_{n+1}|} \right\}^{1/m} \text{sign}(\frac{\tau_n^{x}}{r_{n+1}}).
\]  

(22)

Of all slip systems \( \dot{\gamma}_n^{x} \) and at time \( t_{n+1} \) (for the sake of clarity, the incremental indices \( n+1 \) will be omitted in the remainder of this section), the slip rates and stress components in Eq. (22) are placed in the columns \( \dot{\gamma}_n^{x} \) and \( \tau_n^{x} \), whereas the right-hand side will be referred to as \( \tau_n^{x} \). The column \( \tau_n^{x} \) contains the 6 independent components of the stress measure \( \tau \), resulting in the Schmid stresses \( \tau_n^{x} \) after employing Eq. (8). At a given stress state, the 12 slip rates in \( \dot{\gamma}_n^{x} \) are solved by Newton–Raphson iterations

\[
\Phi(\dot{\gamma}_n^{x}, \tau_n^{x}) = \dot{\gamma}_n^{x} - \Gamma_n^{x} = 0.
\]

(23)

To actually determine the stress column \( \tau_n^{x} \), Eq. (19) is also solved using a Newton–Raphson iteration procedure. With respect hereto, a distinct formulation of the derivatives of the slip rates with respect to the stress components of \( \tau_n^{x} \) (\( d\dot{\gamma}_n^{x}/d\tau_n^{x} \)) is required to construct a consistent tangent. For this purpose, the ansatz is that Eq. (23) must remain satisfied for all variations of \( \tau_n^{x} \)

\[
\frac{d\Phi}{d\tau_n^{x}} = 0,
\]

(24)

with \( 0 \) the zero matrix \((12 \times 6)\). This can be expanded to

\[
\frac{d\Phi}{d\tau_n^{x}} = \left( \frac{\partial \Phi}{\partial \tau_n^{x}} \right) + \left( \frac{\partial \Phi}{\partial \tau_n^{x}} \right) \frac{d\dot{\gamma}_n^{x}}{d\tau_n^{x}} = 0.
\]

(25)

The derivatives \( d\dot{\gamma}_n^{x}/d\tau_n^{x} \) are released through rearrangement of this linear equation

\[
\frac{d\dot{\gamma}_n^{x}}{d\tau_n^{x}} = - \left( \frac{\partial \Phi}{\partial \tau_n^{x}} \right)^{-1} \frac{\partial \Phi}{\partial \tau_n^{x}}.
\]

(26)

Now, the system can be solved for both the slip rates \( \dot{\gamma}_n^{x} \) and the slip system resistances. Recapitulating, this iteration procedure (for solving the slip rates and resistances) is performed for each stress state, i.e., during each iteration of the Newton–Raphson procedure of the overall system of equations.

3. Intragranular decomposition

3.1. Modified Taylor approach

As an interaction strategy for relating the mechanical behaviour of the microstructure to macroscopically imposed deformation conditions, following Taylor’s model, the
stress at each macroscopic continuum material point is determined by the averaged response of the microstructural constituents comprising that material point.

However, the classical Taylor assumption enforces the deformation of each individual grain in a material point to be uniform and equal to the macroscopic deformation, disregarding any interactions between grains or inside grains. In reality though, the intragranular deformation in general is heterogeneous, and at the grain boundaries, equilibrium of mechanical forces must hold (Becker and Panchanadeeswaran, 1995). Therefore, in the presented intermediate model, these discrepancies are partially amended by relaxing the Taylor approach.

Each grain is fictitiously subdivided into a core and several grain boundary fractions, represented by a single crystal and bi-crystals, respectively. This subdivision is shown two-dimensionally in Fig. 2. The crystal lattice orientation of the bi-crystal fragment situated next to the core (interior-side part “i”) initially resembles that of the core, whereas the exterior-side part “e” of the bi-crystal has the same initial crystallographic orientation as its neighbouring crystal.

At the end, for each grain “k”, the Cauchy stress $\sigma^k$ is computed by volume-averaging the stresses of each of the constituents, i.e., the stress in the single crystal core $\sigma^{k,c}$ and the stresses in the $N^k_b$ bi-crystals $\sigma^{k,b}$

$$\sigma^k = \vartheta \sigma^{k,c} + (1 - \vartheta) \frac{1}{N^k_b} \sum_{b=1}^{N^k_b} \sigma^{k,b},$$

where $\vartheta$ (0 $\leq \vartheta \leq 1$) is the volume fraction of the crystal core (cf. Eq. (35) in Section 4). In this fashion, the contribution of each bi-crystal of grain $k$ is weighted equally. Finally, in parallelism to Asaro and Needleman (1985), for the determination of the macroscopic stress, all grains are assumed to be equally sized.

$$\bar{\sigma} = \frac{1}{N_k} \sum_{k=1}^{N_k} \sigma^k,$$
where \( N_k \) is the number of grains with an independent crystallographic orientation considered in the material point under investigation. In the following, the attention is focussed on the entire crystal, including the core and the associated bi-crystals (the superscript “\( k \)” is omitted as from now).

Considered more thoroughly, the deformation of the grain interior is still imposed to be uniform and equal to the macroscopic deformation gradient \( \mathbf{F}_c \), in accordance to the classical Taylor assumption

\[
\mathbf{F}_c = \mathbf{F}
\]

(29)

On the other hand, only the average of the two individually uniform deformation gradients of the bi-crystal fragments, \( \mathbf{F}^{b,i} \) and \( \mathbf{F}^{b,e} \), is enforced to equal the macroscopic deformation gradient

\[
f_0^{b,i} \mathbf{F}^{b,i} + f_0^{b,e} \mathbf{F}^{b,e} = \mathbf{F}, \quad f_0^{b,i} + f_0^{b,e} = 1,
\]

(30)

where \( f_0^{b,i} \) and \( f_0^{b,e} \) are the initial volume fractions of the interior and exterior sections of the bi-crystal element “\( b \)”, respectively.

For the calculation of the stress in the crystal core \( \sigma_c \), the relations of Sections 2.2 and 2.3 are to be used. For the computation of the two bi-crystal stresses, \( \sigma^{b,i} \) and \( \sigma^{b,e} \), additional restrictions have to be formulated. In the plane of the interface between the two crystals in the bi-crystal, state variables are enforced to be uniformly distributed, i.e., only variations of quantities perpendicular to the interface are of interest. First, at the bi-crystal interface, the condition of kinematical compatibility must hold, only admitting variations between the deformation gradients \( \mathbf{F}^{b,i} \) and \( \mathbf{F}^{b,e} \) in the direction of the initial outward interface normal \( \mathbf{n}_0 \), cf. Fig. 2. After consideration of Eq. (30), the deformation gradients can be written according to

\[
\mathbf{F}^{b,i} = \mathbf{F} + f_0^{b,e} \mathbf{a} \mathbf{n}_0, \\
\mathbf{F}^{b,e} = \mathbf{F} - f_0^{b,i} \mathbf{a} \mathbf{n}_0
\]

(31)

with \( \mathbf{a} \) an a priori unknown vector. Second, in addition to compatibility, stress equilibrium at the interface in the deformed state is enforced through the condition

\[
(\sigma^{b,i} - \sigma^{b,e}) \cdot \mathbf{n}^b = 0, \quad \mathbf{n}^b = \frac{\mathbf{F}^{-T} \cdot \mathbf{n}_0}{||\mathbf{F}^{-T} \cdot \mathbf{n}_0||}.
\]

(32)

Note that this equation includes the instantaneous interface orientation \( \mathbf{n}_0^b \), whereas in Eq. (31), the initial orientation \( \mathbf{n}_0^b \) is used.

3.2. Time integration

Regarding the time integration, besides solving the Piola–Kirchhoff stresses in both bi-crystal fragments using the approach given in Sections 2.2 and 2.3, the internal deformation gradient variation \( \mathbf{a}_{n+1} \) has to be determined simultaneously. The set of equations is therefore naturally completed by the traction equilibrium condition (32). The entire system of coupled equations is then solved using the Newton–Raphson
iterative procedure. Finally, the bi-crystal stress (at time $t_{n+1}$), as required in Eq. (27), is taken equal to the (uniform) stress of the interior-side part, $\sigma^{bi}$. 

4. Enhanced hardening

The potential existence of heterogeneous intragranular deformations is the point of departure for this section. Within each grain, the deformation incompatibility between the core and the interior bi-crystal parts, sections with initially equal lattice orientations, requires the generation of geometrically necessary dislocations (GNDs). First, the densities of GNDs between the core and each bi-crystal component are determined. Next, in addition to the “conventional” slip resistance $s^2$ in Eq. (10), an extra term is introduced, based on the GND densities.

The evolution of the statistically stored dislocations (SSDs) has no geometric consequences and is recognized as the motive behind the conventional slip system strength $s^2$. From now on this strength will be denoted as $s^2_S$, while the extra term related to the GNDs will henceforth be denoted as $s^2_G$.

4.1. GND density

In this section, the GND densities between the core of a particular grain and one of its bi-crystal boundary elements are scrutinized. The same approach applies to the remaining bi-crystals as well as the other grains in the material point. A measure for the plastic deformation incompatibility is given by Nye’s dislocation tensor (cf. Nye, 1953; Mura, 1987), which is defined as the curl of $F_p$ (Dai, 1997)

$$ A \equiv - (\nabla_0 \times F_p^T)^T. $$

Physically, this tensor can be interpreted as a measure for the closure failure (cumulative Burger’s vector) of the contour enclosing an infinitesimal surface when the inner product of Nye’s tensor with the surface unit normal vector is integrated over that surface. That closure failure is caused by the type and quantity of dislocations piercing the enclosed surface.

As due to the in-plane homogeneity of the bi-crystal interfaces only variations in the direction perpendicular to that interface are considered, in this particular case, Nye’s tensor can be written as a function of the interface normal $n^b_0$ and the gradient of $F_p$ between the core and the bi-crystal (cf. Fig. 3)

$$ A = - \left( n^b_0 \times \frac{\Delta F_p^T}{l} \right)^T, \quad \Delta F_p = F^{bi}_p - F^c_p, $$

with $l$ a length parameter representing the width of the intercrystal dislocation dominated transition zone.

The parameter $l$ is geometrically related to the core volume fraction $\vartheta$ of Eq. (27) and to the grain diameter $d$. Suppose each grain is, for the moment, represented by a sphere with diameter $d$. The centre of the sphere is occupied by the core volume fraction $\vartheta$. According to Eq. (27), the volume of the shell surrounding the core is
attributed to the bi-crystals. The thickness of that shell represents the grain boundary region

\[ l = \left(1 - \sqrt{\vartheta}\right) \frac{d}{2}, \quad (35) \]

Note that this relation also holds for cubical grain representations.

It is assumed that this region stores the geometrically necessary dislocations, i.e., the variation of \( F_p \) is accommodated in this region only. At a constant \( \vartheta \), \( l \) varies proportional to the grain size. The GNDs are then stored in an increased volume for larger grains, which will lower the free energy of the grain. Other choices in this respect are varying \( \vartheta \) as a function of \( d \) while keeping \( l \) fixed or a more sophisticated ansatz incorporating the deformation history. However, there are no clear physical arguments to support these choices. Furthermore, it turns out that these alternative choices do not show a Hall–Petch-like behaviour as well as the chosen approach with a constant core fraction.

Once Nye’s tensor has been computed, the related dislocation densities are determined by representing Nye’s tensor as the cumulative contribution of all 18 (12 edge and 6 screw, cf. Kubin et al., 1992) types of GND densities \( \rho^\zeta \) following the approach of Arsenlis and Parks (1999)

\[ \lambda_0 = \sum_\zeta \rho^\zeta_0 b^\zeta_0 t^\zeta_0, \quad (36) \]

where \( b^\zeta_0 \) and \( t^\zeta_0 \) are the (initial) Burgers and tangent vector of each dislocation type \( \zeta \), respectively. Because of the fact that Nye’s tensor only has nine independent components, various combinations of dislocation densities may compose the incompatibility of plastic deformation between the core and the boundary. Without knowledge of the crystallographic dislocation density evolution or additional constraints, it is impossible to determine the exact dislocation structure. Two procedures have been proposed by Arsenlis and Parks (1999) to find a lower bound of GND densities accommodating a given Nye tensor. The approach of minimizing the sum of the squares of the dislocation densities is favoured over the minimization of the total dislocation line length in the present work.
The motion of gliding dislocations on a slip plane is obstructed by forest dislocations piercing that slip plane. The GNDs contribute to this crystalline strengthening by creating additional pile-ups and by augmenting the forest dislocation density. The strengths and densities of those obstacles depend on the dislocation densities in all directions and their mutual interactions. Through a set of interaction coefficients \( A^\xi \) and the dislocation density magnitude \( |\rho^\xi| \), the effective density of point obstacles to mobile dislocation motion on slip system \( \alpha \) can be determined, as proposed by Franciosi and Zaoui (1982) (as the dislocation profile on the slip systems is unknown, the interaction coefficients are solely based on the dislocation Burgers vectors). The enhanced slip system strength \( s^\alpha \) is related to the square root of that effective density following Ashby (1970)

\[
s^\alpha_G = c \mu b \sqrt{\sum_\xi A^\xi |\rho^\xi|},
\]

where \( c \) is a constant, \( \mu \) is the shear modulus and \( b \) is the length of the Burger’s vector.

Information on the densities of SSDs is only implicitly available through the slip system strength \( s^\alpha_S \). Hence, individual densities of SSDs, for the 18 dislocation types, is not possible. This makes a direct addition of the densities of SSDs and GNDs in an explicit fashion quite ambiguous. Alternatively, the overall slip strength \( s^\alpha \) is taken as a coupling between the corresponding contributions of both dislocation types

\[
s^\alpha = (s^\alpha_S)^p + (s^\alpha_G)^p \]

where \( p = 1 \) represents a straightforward addition of both strengths and \( p = 2 \) implies summing the attributive dislocation densities in an effective way. In this work, both choices are reviewed.

5. Numerical results

The presented model, including enhanced work hardening by GNDs, has been implemented in order to simulate the stress–strain behaviour of a FCC polycrystal composition during uniaxial tension for different grain sizes. The grain size dependence of the flow stress, also known as the Hall–Petch effect (cf. Eq. (1)), in this context is treated as the result of the increase of GND densities for maintaining lattice compatibility with decreasing grain sizes Ashby, 1970). Consequently, small grained polycrystalline materials exhibit more resistance to an applied deformation than larger grained ones.

The computations are compared to numerical and experimental results found in literature. First, the constitutive response is confronted with detailed finite element computations on polycrystalline copper by Arsenlis and Parks (2000). The finite element mesh used by Arsenlis and Parks, consisting of 27 randomly oriented cubic grains, is transformed into a morphologically similar material point representation, using 27 single crystals, having similar lattice orientations and being arranged in the same spatial directions, with 54 bi-crystals. This representation is (partly) depicted in Fig. 4. In
both simulations, uniaxial tension is applied in the $z$-direction. The strain rate is fixed at $0.001 \text{s}^{-1}$.

For copper, many contradictory experimental results exist, in which quite often the Hall–Petch relation fails as a result of the intersection of stress–strain curves of fine grained copper with the stress–strain curves of coarse grained copper. This effect is often attributed to texture developments. Therefore, in this work, the experimental findings of Hansen (1979) have been chosen for comparison with the simulations. In that work, parallel stress–strain curves are determined, which is achieved by preparing large-grained specimens by reducing the amount of deformation prior to recrystallization. Moreover, the ratio between the specimen diameter and the grain size was taken to be larger than $15$ to minimize the effect of surface grains. Hansen performed tensile tests on polycrystalline copper strips with average in-plane grain diameters of $14$, $33$ and $220$ $\mu$m.

In the simulation, the diameter ($d$ in Eq. (1)) is varied similar to the experiments ($14$, $33$ and $220$ $\mu$m), whereas the crystallographic orientations are left identical. The core volume fraction is set constant to $\vartheta = 0.5$ (Evers et al., 2000). The initial internal bi-crystal fractions are taken according to $f_{0}^{b,i} = f_{0}^{b,e} = 0.5$ for each bi-crystal “b”. The constitutive parameters are given in Table 1.

The dislocation interaction coefficients of the matrix $A^{\alpha \gamma \beta}$ depend on the interaction types between dislocations on different slip systems, as documented by Franciosi and Zaoui (1982). They classify those interactions according to whether the dislocations belong to the same slip system (self-hardening, interaction coefficient $a_0$), belong to coplanar slip systems or form Hirth locks (interaction coefficient $a_1$), form glissile junctions (interaction coefficient $a_2$) or Lomer–Cottrell locks (interaction coefficient $a_3$), with $a_0 \leq a_1 \leq a_2 \leq a_3$. Finally, the initial density of GNDs is taken to be zero on all slip systems and in all bi-crystals of the material point.

In the numerical procedure, the stresses in the single crystal interiors and in each half of all bi-crystals are computed independently. Successively, the stress of each of the 27 grain compositions ($\sigma^k$) is determined by the evaluation of Eq. (27), and conventional Taylor averaging of all compositions by Eq. (28) (since, in this example, all grains are
Table 1
Constitutive parameters of copper (Dai, 1997; Arsenlis and Parks, 2000)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Magnitude</th>
<th>Units</th>
<th>Used in</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s modulus</td>
<td>$E$</td>
<td>144</td>
<td>GPa</td>
<td>Eq. (6)</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td>$v$</td>
<td>0.33</td>
<td>—</td>
<td>Eq. (6)</td>
</tr>
<tr>
<td>Reference plastic strain rate</td>
<td>$\dot{\gamma}_0$</td>
<td>0.001</td>
<td>s$^{-1}$</td>
<td>Eqs. (7) and (22)</td>
</tr>
<tr>
<td>Strain rate sensitivity</td>
<td>$m$</td>
<td>0.012</td>
<td>—</td>
<td>Eqs. (7) and (22)</td>
</tr>
<tr>
<td>Initial slip resistance</td>
<td>$\tau_0$</td>
<td>8</td>
<td>MPa</td>
<td>Eq. (10)</td>
</tr>
<tr>
<td>Latent hardening ratio</td>
<td>$q$</td>
<td>1.4</td>
<td>—</td>
<td>Eq. (11) (in $q^{2\beta}$)</td>
</tr>
<tr>
<td>Hardening parameter</td>
<td>$h_0$</td>
<td>250</td>
<td>MPa</td>
<td>Eq. (12)</td>
</tr>
<tr>
<td>Saturation value</td>
<td>$s_\infty$</td>
<td>190</td>
<td>MPa</td>
<td>Eq. (12)</td>
</tr>
<tr>
<td>Hardening rate exponent</td>
<td>$a$</td>
<td>2.5</td>
<td>—</td>
<td>Eq. (12)</td>
</tr>
<tr>
<td>Adjustable parameter</td>
<td>$c$</td>
<td>0.3$^a$ and 0.7$^b$</td>
<td>—</td>
<td>Eq. (37)</td>
</tr>
<tr>
<td>Shear modulus</td>
<td>$\mu$</td>
<td>41.5</td>
<td>GPa</td>
<td>Eq. (37)</td>
</tr>
<tr>
<td>Burger’s vector length</td>
<td>$b$</td>
<td>0.25</td>
<td>nm</td>
<td>Eq. (37)</td>
</tr>
<tr>
<td>GND interaction coefficient</td>
<td>$a_0$</td>
<td>0.06</td>
<td>—</td>
<td>Eq. (37) (in $A^{2\xi}$)</td>
</tr>
<tr>
<td>GND interaction coefficient</td>
<td>$a_1/a_0$</td>
<td>5.7</td>
<td>—</td>
<td>Eq. (37) (in $A^{2\xi}$)</td>
</tr>
<tr>
<td>GND interaction coefficient</td>
<td>$a_2/a_0$</td>
<td>10.2</td>
<td>—</td>
<td>Eq. (37) (in $A^{2\xi}$)</td>
</tr>
<tr>
<td>GND interaction coefficient</td>
<td>$a_3/a_0$</td>
<td>16.6</td>
<td>—</td>
<td>Eq. (37) (in $A^{2\xi}$)</td>
</tr>
</tbody>
</table>

The parameter $c$ is determined in this analysis; the coefficients $a_0, a_1, a_2$ and $a_3$ are entries in the dislocation interaction matrix $A^{2\xi}$, which is documented by Franciosi and Zaoui (1982) and quantified for copper by Cuitiño and Ortiz (1992).

$^a$combined with $p = 1$ in Eq. (38).

$^b$combined with $p = 2$ in Eq. (38).

equally sized) yields the macroscopic stress in the material point, $\bar{\sigma}$, which is evaluated next.

In the evaluation, two options are examined. First, the contributions of the SSD and GND densities are combined by linear addition of their corresponding slip system strengths, $s^z_S$ and $s^z_G$ in Eq. (38), respectively. Second, following the finite element simulations of Arsenlis and Parks, the choice of effectively adding SSD and GND densities is regarded, which is reflected by setting $p = 2$ in Eq. (38). This can be stated when conferring the relation between strength and dislocation density in Eq. (37), which is also implicitly assumed for the case of SSDs, where the relation at issue actually originates from. Correspondence to the experiments (Hansen, 1979) could be achieved by the adjustment of a single parameter ($c$ in Eq. (37)) in either case of dislocation strength or density addition.

5.1. Stress–strain behaviour

The simulated and experimentally determined uniaxial stress–strain curves are given in Fig. 5a and b. In both figures, no considerable grain size effect is predicted at the onset of yielding, which is not in line with experimental findings in general. This observation is attributed to the numerical assumption that no initial GND densities are present in the material, which contradicts with reality, as during the processing of the polycrystalline material, certain amounts of GND densities are introduced (i.e.,
next to the GNDs comprising the grain boundaries themselves). Furthermore, from the figures, it can be concluded that both the detailed simulations of Arsenlis and Parks and the simulations encompassing the summation of the dislocation densities show an almost perfect agreement with the experimentally observed grain size dependent behaviour, whereas the simulations encompassing the dislocation strength addition show a small deviation for the large grained specimen. Nevertheless, the intragranular inhomogeneities between the core and the bi-crystals as effectuated by the adapted Taylor assumption bring about a similar effect as the inhomogeneity between the finite elements of the two regions in the case of the discretized grains when, for both cases, the enhanced hardening approach is applied. Therefore, the presented advanced polycrystal model appears to be an adequate alternative for the fully discretized finite element simulations for applications where the (macroscopic) length scale at issue is large with respect to the size of the individual grains (i.e., when such a polycrystal approach is valid).

5.2. Hall–Petch parameters

The magnitude of $\sigma_0(\varepsilon)$ in the Hall–Petch equation (38) can be recovered by performing an additional simulation. In that simulation, by excluding $s_G$ from Eq. (38), virtually, grains of infinite dimension are modelled and $\sigma_0(\varepsilon)$ is determined.

The two remaining Hall–Petch parameters, i.e., the Hall–Petch slope $k$ and the exponent $n$ (cf. Eq. (1)) are determined in such a way that the total accumulated difference between the simulated stress–strain curves and the curves following from the Hall–Petch relation is minimized in a least squares sense. For this, it is assumed that $n$ is a constant and that $k$ may vary as a function of the strain $\varepsilon$. This strain domain is discretized, using $N$ supporting values $\varepsilon^i (i = 1, 2, \ldots, N)$, and at each point $\varepsilon^i$, the difference between the stress $\sigma_{\text{HP}}^i$ according to Eq. (1) and the simulated uniaxial stress
Fig. 6. Simulated stress–strain curves of all diameters (solid lines) and the Hall–Petch fits (cf. the marks) to that data, where the Hall–Petch parameters $n$ and $k$ are determined through minimization of (39).

(a) Results using the assumption of SSD and GND strength addition. (b) Results using the assumptions of SSD and GND density addition.

\[
\sigma' \left( \varepsilon \right) = \min_{\{n,k\}} \left\{ \sum_{j=1}^{3} \sum_{i=1}^{N} \frac{\left( \sigma_{\text{HP}}^j \left( d^j \right) - \sigma' \left( d^j \right) \right)^2}{\left( \sigma' \left( d^j \right) \right)^2} \right\}^{1/2}.
\]

Accordingly, $N$ values of the Hall–Petch slope $k^j$ as well as the constant $n$, which together with $\sigma^j_0$ and the fixed diameters $d^j$ (14, 33 and 220 $\mu$m) basically determine $\sigma_{\text{HP}}^j \left( d^j \right)$, are simultaneously quantified through the minimization.

For the cases of dislocation strength addition versus dislocation density addition, the resulting $n$ reads 0.50 and 0.94, respectively. These values originate from the way in which the geometric effects are incorporated into the slip system resistance (and, correspondingly, the flow stress), i.e., the incorporation of $s_G^2$ in $s^2$ according to Eq. (38). The reason behind this is the intrinsic diameter dependence of $s_G^2$ through Eqs. (34)–(37). Through these one could say physically based equations, the influence of the diameter on the constitutive behaviour is retrieved. Furthermore, Arsenlis and Parks determined $n$ to be in the range of 0.88 to 0.93 in their simulations incorporating dislocation density addition.

In the Figs. 6a and b, for the assumptions of SSD and GND strength addition and density addition, respectively, the agreement of the Hall–Petch relation using the corresponding computed Hall–Petch parameters with the simulated stress–strain curves is shown. In both cases, the Hall–Petch relation is perfectly suited to describe the grain size dependent response.

For comparison, the Hall–Petch parameters based on the experimental results by Hansen also have been computed. After minimization of expression (39), the Hall–Petch exponent is determined to be 0.80. Based hereon, the stress–strain curves are constructed for all diameters such as they are predicted by the Hall–Petch relation. These curves are compared to the experimental data in Fig. 7.
Fig. 7. Comparison of the experimental data of Hansen (cf. the marks) to the curves which are computed by applying the computed parameters $n$ and $k$ to the Hall–Petch relation for all diameters (solid lines).

From the present analysis, it can be concluded that the determination of the actual Hall–Petch exponent $n$ is very sensitive to minor changes in the material response. This also explains why various values of the exponent can be found in the literature for the same material, but possibly with minor changes in their processing history. The best correspondence with the particular experimental findings of Hansen is achieved using the assumption of summing the SSD and GND densities ($p = 2$ in Eq. (38), cf. Fig. 5).

6. Conclusion

A local plastic strain gradient dependent crystal plasticity model has been developed, describing the grain size dependent behaviour of a polycrystal material (i.e., an aggregate of grains is considered attributed to a material point). Intragranular incompatible deformations, which arise as a result of the consideration of grain boundaries (represented by bi-crystals), are used to determine the amount of additional –geometrically necessary– dislocations. The density of these dislocations determines the amount of enhanced hardening through the formation of additional obstacles, obstructing the propagation of slip.

As the intragranular heterogeneous deformation is intrinsically related to the grain size, so is the magnitude of the enhanced hardening term. Furthermore, the conventional slip system hardening by the statistically stored dislocations is described by a system of phenomenological equations, covering the effects of both self and latent hardening. Both SSD and GND slip resistances are combined in two different ways, one in which they are simply summed and one in which, implicitly, their accompanying forest dislocation densities are added.

Both approaches of the presented local polycrystal material model have been compared to full-scale finite element simulations considering the addition of dislocation densities and, moreover, to experimentally determined tensile curves dealing with
several (average) grain sizes. For these simulations, an analogous representation of the finite element mesh with respect to crystallographic and morphological orientations has been applied in the polycrystal material point representation. The resulting grain size dependent tensile curves, as computed by the enhanced Taylor approach at hand, agree well with the finite element computations and with the experimental data. The agreement is almost perfect for the case of dislocation density addition and good for the case of dislocation strength addition. Therefore, the polycrystalline crystal plasticity model is found to be a worthy substitute for the full-scale finite element model from a computational point of view.

It has been shown that the applied model is well suited to describe the grain size effect in a physically interpretable manner (i.e., without explicitly introducing grain size dependency in a flow stress relation). Moreover, additionally, the morphological texture can be incorporated through the orientation of the grain boundaries and their mutual weight (Evers et al., 2000). Therefore, it is believed to be one of the most sophisticated models available nowadays at the polycrystal level.

The present model focused on the elaboration of a polycrystalline model that includes a physically based dependence on the grain size. In order to make well founded choices concerning the combination of several dislocation types, a crystal plasticity formulation which is completely based on dislocation densities should yet be developed. This gives also the opportunity to consider substructuring inside the grains, which is believed to dominate strain hardening at intermediate strains.

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References


