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Crystal plasticity and hardening: a dislocation dynamics study

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Abstract

Following the publication of several seminal studies, discrete dislocation dynamics has become well-established as a means of analysing the response of ductile crystals and polycrystals to mechanical loading. Developments undertaken by different authors have followed two principal directions: (i) the use of simple 2D formulations that do not seek to capture correctly the details of slip geometry, but allow some insight to be developed into the trends and relationships, and (ii) large scale 3D simulations seeking to represent correctly the geometry of dislocation segments, and their spatial distribution and interaction. The former is computationally inexpensive and fast, but fails to capture the effects of grain orientation. The latter is associated with large overheads in terms of the computational effort. The purpose of the present study is to propose and develop an intermediate level approach, whereby the geometry of the crystal slip is captured to a greater degree, while computational difficulty is kept to a minimum. The results are analysed in terms of the dependence of yield stress and cyclic hardening on the crystal orientation and dislocation interaction with each other and with the grain boundaries.

Keywords: Crystal plasticity, discrete dislocation dynamics, crystal orientation, hardening

1. Introduction

The mechanical behaviour of modern engineering alloys can be studied at a multitude of different scales. At each particular scale the behaviour arising from the lower scales must be captured via a set of constitutive rules. At the macroscopic scale (the classical solid mechanics continuum) the material properties are interpreted as an average over a large number of grains within a polycrystal. Some aspects of the material's mechanical behaviour, such as elastic response, yield, kinematic and isotropic hardening etc.., can be efficiently captured by continuum models.

At the next lower scale, the material behaviour at the scale of individual grains within the polycrystal needs to be considered. Observed material strengthening due to grain refinement (after Hall[1] and Petch[2]) reflects the importance of strain gradients that arise in polycrystalline metals due to the inhomogeneous deformation behaviour within and between neighbouring grains. Ashby[3] pointed out the fundamental difference between the homogeneous plastic deformation that can be accommodated by arbitrarily uniform distributions of dislocations (statistically

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stored dislocations, SSD) and the particular nature of the dislocation distributions required to accommodate plastic strain gradients (geometrically necessary dislocations, GND).

Strain-gradient crystal plasticity concepts are a widely accepted means of studying grain level material behaviour. A physically intuitive approach was developed by Busso et al.[4], who introduced strain gradient effects directly into the evolution laws for the internal slip system state variables. This model has provided an important physical insight into the effects of microstructure on the macroscopic response, including rate-independent plastic deformation and visco-plasticity in both single crystal and polycrystalline materials (Busso and Cheong[5], Meissonnier et al.[6]).

The inelastic deformation in polycrystalline engineering metallic alloys at room temperature and at quasi-static rates occurs largely by dislocation glide. Dislocation dynamics simulations have become a well accepted means of studying the mechanics of dislocation interaction and their effects on crystal level deformation. The development of dislocation dynamics models has thus far followed two principal directions: (i) the use of simple 2D formulations that do not seek to capture correctly the details of slip geometry, but allow some insight into the trends and relationships, and (ii) large scale 3D simulations seeking to represent correctly the geometry of dislocation segments, their spatial distribution, and their interactions.

Large-scale 3D computations have been presented by Devincre and Kubin[7] in the form of a 3D lattice-based dislocation dynamics model, where dislocations are considered to move over a prescribed mesh of material points. This model has been used extensively to investigate the strengthening effect of dislocation reactions during stage I, II and III loading of single crystals. An alternative 3D dislocation dynamics framework has been proposed by Cai, Bulatov, Arsenlis and co-workers[8,9]. They consider dislocations as line defects, discretised into segments, which propagate in an elastic continuum. Dislocation motion is governed by a mobility function capturing the effects of lattice orientation, solute elements, hydrostatic stress etc. This model has been implemented in the ParaDiS (Parallel Dislocation Simulator) code. A drawback of both frameworks, that proposed by Devincre and Kubin and that due to Arsenlis et al.[9], are that vast computational resources are required to run these simulations. For all but small demonstration problems, computation demands quickly outgrow normal lab computing resources.

An alternative method was chosen by Van der Giessen and Needleman[10]. They considered a 2D setup where edge dislocations glide along three pre-defined slip systems. The dislocations are introduced from a number of randomly distributed sources. Their motion is governed by a mobility function and the interactions are prescribed by a set of constitutive rules. The boundary value problem is solved by a finite element model providing a stress field which is superimposed on the dislocation stress field to produce the total stress field at each time step. To increase the generality of this framework, Deshpande et al.[11] proposed an extension to finite deformation and rotations, and Benzerga et al.[12] proposed some extended constitutive rules to mimic 3D phenomena, like Frank-Read source formation and annihilation, and dislocation line tension. This 2D dislocation dynamics framework has been applied to a wide range of problems. Bittencourt et al. [13] presented a comparison with the continuum crystal visco-plasticity model proposed by Gurtin[14] and discusses the importance of the inherent length scale formed by the blocked dislocation boundary layer at an interface. Nicola et al.[15] report similar observations in the case of single and polycrystalline thin films. Size effects in free standing single crystals and polycrystals and the influence of specimen boundary conditions have also been investigated by Deshpande et al.[16] and Balint et al.[17]. Finally, Widjaja et al.[18] have used the dislocation framework to model micro-indentation, and Deshpande et al.[19] have modelled fatigue crack growth.

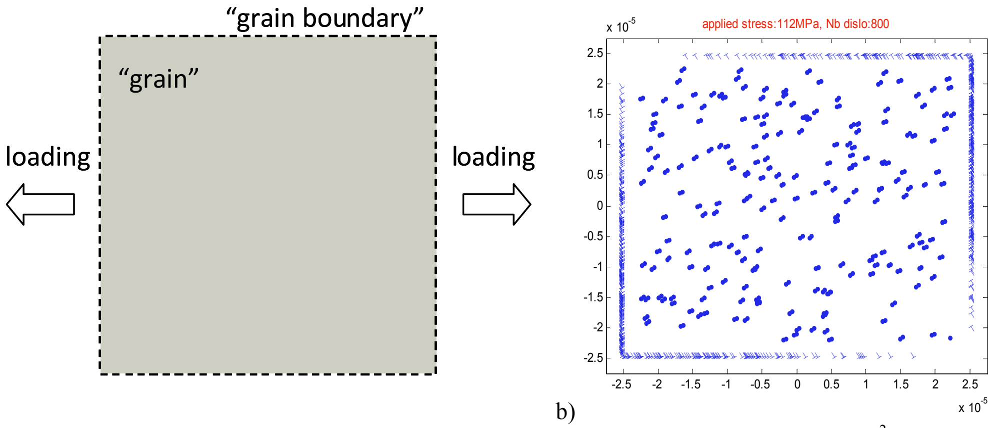
The attractiveness of this model lies in the fact that, although it largely neglects the complexities of 3D dislocation interactions, it still captures successfully the fundamental trends of material behaviour due to dislocation motion. Due to its 2D nature the model itself is comparatively straightforward to implement and computationally inexpensive. Thus far a limitation of the model has been that the prescription of slip systems has been rather arbitrary, consisting of three slip systems separated by 60º. Here we propose an extension that takes into account a more realistic distribution of slip systems based on the projection of 3D crystal slip systems for an FCC metal onto the simulation plane. This model is used to study the lattice orientation-dependent yield and cyclic deformation.

2. Dislocations motion and plasticity

Dislocation motion simulation in this paper follows the framework described by van der Giessen and Needleman[10]. In order to describe the slip planes in which edge dislocations can glide, a projection into the simulation plane of the 3D slip planes is carried out. For an fcc crystal, four distinct slip planes exist: (111), $(\bar{1}11)$, $(1\bar{1}1)$, $(11\bar{1})$. The rotation matrix **R** describes the transformation of any vector from the crystal coordinates to the lab reference frame. Hence, the normal to a crystal slip plane $\boldsymbol{n}_r$ in the lab reference frame is given by: $\boldsymbol{n}_r = \boldsymbol{R} \cdot \boldsymbol{n}$.

Dislocations are constrained to glide along the intersection of the simulation plane with each slip plane. Initially the simulation volume is free of dislocations and only a fixed number of randomly distributed Frank-Read sources is present, equally divided between slip systems. To determine if a source can emit a pair of edge dislocations, the local stress is projected onto the slip direction to determine the shear traction on the source. If the shear traction at a source reaches the critical value of τ_{nuc}, a pair of dislocations of the opposite sign is emitted.

Dislocations motion is caused by the Peach-Koehler force. In our model, dislocations are allowed to move freely until they reach a grain boundary, where they become permanently pinned. The grain boundary is taken to coincide with the boundary of the simulation area. Total strain is found as $\varepsilon = \varepsilon^{el} + \varepsilon^{pl}$, where the grain-average plastic strain due to the dislocation passage is computed as $\varepsilon^{pl} = b \cdot l / A$, where b is Burgers' vector magnitude, l is the path length of the dislocation, and A is the area of the simulation box. Figure 1(a) illustrates the problem set up, and Fig.1(b) the dislocation distribution after a remote tensile stress has been applied and equilibrium was reached.



a) b)

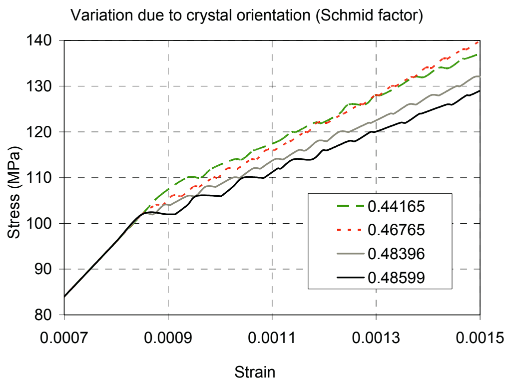
Figure 1: (a) Schematic diagram of the "grain" problem. (b) Dislocation distribution in a grain (50×50μm^2) after the application of a horizontal tensile remote stress of 110 MPa. Frank-Read sources are represented by pairs of dots.

3. Results and discussion

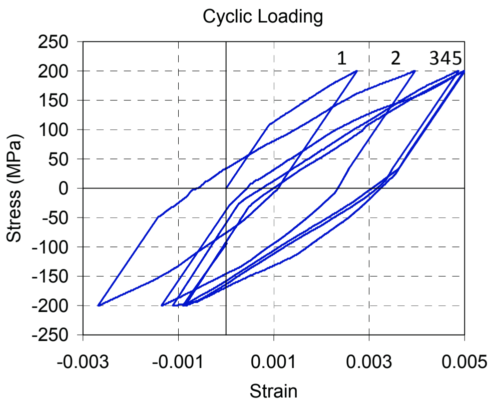
To probe the variation of the deformation response with lattice orientation, stress-strain curves were computed for a number of different lattice orientations (Figure 2a). It is apparent that the onset of yield occurs at different applied stress levels depending on the lattice orientation. The post-yield stress-strain curve (strain hardening) also shows a dependence on the lattice orientation. Thus, the model captures the anisotropic plastic properties of single crystals, and hence the orientation dependence of the uniaxial deformation response.

The orientation dependence of the yield stress can be understood in terms of the maximum resolved shear stress acting on any particular glide plane. This is the dependence captured by the Schmid factor. The actual response also depends on the presence of dislocations prior to yield and the distribution of dislocation sources and obstacles. The post-yield stress-strain response is governed by the availability of dislocation sources and ability of the dislocations to move. If a slip system is "starved" of dislocation sources, it will exhibit a higher strength, whilst a slip system with a large number of sources will show early yield. After the initiation of plastic deformation dislocations propagate through the grain until they become pinned at the grain boundaries. As the number of dislocations on a given slip system increases, the back stress exerted on the source increases, and a higher external stress is required for the emission of further dislocations. For further plastic deformation, either a higher external stress has to be applied, or a yield on an alternative, "softer" slip system has to occur.

Figure 2(b) shows the behavior of a grain under cyclic loading. Isotropic and kinematic hardening are well identifiable, the former corresponding to the yield surface expansion, and the latter describing the displacement of the yield surface centre. The kinematic hardening is closely related to the so-called "Bauschinger effect", manifested in the fact that a material does not have the same yield stress value in compression after tensile loading as in simple tension. Finally, we observe the saturation of the cyclic hysteresis shape. Under initial elastic loading, dislocations neither move nor can be created. When yield is reached, sources start creating new dislocations and these start moving, so that grain yielding is observed. Dislocation pinning at grain boundary results in lack of reversibility that explains the increase in the back stress, and the observed Bauschinger effect. Cycle stabilization occurs when the dislocation arrangement is reached such that any new dislocations generated in one half of the cycle annihilate again in the second half of the cycle, and the overall number of dislocations remains constant.



(a)



(b)

Figure 2. Grain stress-strain curves: (a) monotonic tension for different Schmid factors (as in legend). (b) cyclic (as numbered).

4. Conclusions

In this paper we presented a simple 2D dislocation dynamics simulation that is a development of the van der Giessen and Needleman[10] model. The approach was extended to reflect better the effect of lattice orientation. For monotonic straining, the model shows orientation-dependant yield and plastic hardening. In the case of cyclic loading the stress-strain curve approaches a stabilized cycle after initial ratcheting, capturing both kinematic and isotropic hardening effects. Promising for future developments, even this simple description appears capable of reproducing some key aspects of deformation behaviour of crystals observed experimentally.

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