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# A discrete dislocation plasticity analysis of grain-size strengthening

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## Abstract

The dependence of shear yield strength on grain size is analyzed using discrete dislocation dynamics. Plastic deformation is modeled through the motion of edge dislocations in an elastic solid. The lattice resistance to dislocation motion, dislocation nucleation, dislocation interaction with obstacles and dislocation annihilation are incorporated through a set of constitutive rules. Grain boundaries are modeled as impenetrable to dislocations. Single slip is assumed within each grain and a checkerboard-like arrangement of grains is used as a unit cell for the polycrystal. Doubly-periodic pure shear calculations are carried out for planar polycrystals with grain sizes in the range  $0.2 \mu\text{m} \leq d \leq 5 \mu\text{m}$  and for two values of initial dislocation source density that differ by an order of magnitude. The offset flow strength varies with grain size,  $d$ , as  $d^{-n}$ , with  $n = 0.40$  or  $n = 0.45$ , depending on source density. The value of the offset flow strength is higher for the low source density polycrystal. Furthermore, for each initial source density, the flow strength was found to scale roughly with dislocation density.

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## 1. Introduction

Hall [1] and Petch [2] correlated the yield strength in mild steel with the inverse square root of grain size:

$$\tau = \tau_0 + kd^{-1/2}. \quad (1)$$

A variety of models have been proposed to account for the grain-size dependence in Eq. (1). Eshelby et al. [3] and Hirth and Lothe [4] proposed that dislocation pile-ups at grain boundaries scale with the grain size,  $d$ , and that stress concentrations associated with a continuous distribution of dislocations in these pile-ups give rise to Eq. (1). Saada [5] has noted that the stress concentrations associated with a pile-up of discrete dislocations may not give rise to Eq. (1). Another model draws on the scaling of flow stress with dislocation density [6] in the form:

$$\tau = \tau_0 + c\rho_{\text{dis}}^{1/2}. \quad (2)$$

Given that the plastic strain,  $\gamma^p$ , scales as

$$\gamma^p \propto b\bar{x}\rho_{\text{dis}}, \quad (3)$$

where  $\bar{x}$  is the mean free path of a dislocation, Eqs. (2) and (3) combine to give the Hall-Petch scaling of the flow strength Eq. (1) at a given value of the plastic strain  $\gamma^p$ , presuming that  $\bar{x}$  scales with the grain size  $d$ . Hirth [7] proposed a model to account for experimentally observed variations in the Hall-Petch exponent by assuming the polycrystal to be a composite microstructure of grain-core regions of radius  $r$  surrounded by hard grain-boundary regions with thickness  $a$ . Using this model and plastic incompatibility concepts, Ashby [8], Hirth [7] obtained the scaling  $\tau \propto d^{-1}$ .

Biner and Morris [9,10] performed two dimensional discrete dislocation plasticity simulations to investigate the Hall-Petch effect. They allowed for dislocation nucleation in the grains in [9] and only at the grain boundaries in [10]. A limited range of source densities was considered and it was concluded that the source density and location have a negligible effect on the Hall-Petch relation. The simulations in [9,10]

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indicated that dislocation pile-ups at the grain boundaries are primarily responsible for the Hall-Petch effect.

Here, we report on calculations of pure shear for planar polycrystals for two initial source densities that differ by an order of magnitude. For each source density, the dependence of offset flow strength on grain size is investigated.

## 2. Polycrystalline discrete dislocation plasticity formulation

The single crystal formulation of Van der Giessen and Needleman [11] is extended to polycrystals and briefly described here. Plane strain conditions are assumed and grains are elastically isotropic with Young's modulus  $E = 70$  GPa and Poisson's ratio  $\nu = 0.33$ . Plasticity originates from the motion of edge dislocations in the  $x_1 - x_2$  plane. Each square grain of side length  $d$  contains a single slip system having slip planes oriented at an angle  $\phi$  with respect to the  $x_1$  axis on which edge dislocations, with Burger's vector  $b$ , can nucleate and glide.

Initially, the polycrystal is stress and dislocation-free. Dislocation sources are randomly distributed on slip planes spaced apart by  $100b$ , with density  $\rho_{\text{nuc}} = 20$  or  $200 \mu\text{m}^{-2}$ . Subsequently, these two cases are referred to as the low (LSD) and high (HSD) source density cases, respectively. Each source is randomly assigned a nucleation strength,  $\tau_{\text{nuc}}$ , from a Gaussian distribution with average 50 MPa and standard deviation 10 MPa. Dislocation nucleation occurs when the resolved shear stress at a source is greater than the nucleation strength  $\tau_{\text{nuc}}$  for the duration of the nucleation time,  $t_{\text{nuc}} = 10$  ns. Dislocation glide is taken to be drag controlled, with zero Peierls stress, so that the velocity of dislocation  $I$  is computed directly from the Peach-Koehler force as  $v^{(l)} = f^{(l)}/B$ , where the drag coefficient,  $B$ , has the value  $10^{-4}$  Pa s. In addition, the dislocations can get pinned at point obstacles randomly distributed in the grains with density  $\rho_{\text{obs}} = 40 \mu\text{m}^{-2}$  for both the LSD and HSD cases. These obstacles release dislocations when the Peach-Koehler force on the obstacle exceeds  $b\tau_{\text{obs}} = 150$  MPa. When two dislocations of opposite sign come closer to each other than the specified annihilation distance,  $6b$ , they are removed from the simulation. Lastly, the grain boundaries are taken to be impenetrable to dislocations.

The material is assumed to consist of a doubly periodic array of square unit cells of side  $L = pd$ , where  $d$  is the grain size and  $p$  the number of grains along a side of the unit cell. The unit cell is subject to pure shear, prescribed through the displacement boundary condition:

$$\Delta u_i = \bar{\epsilon}_{ij} \Delta x_j, \quad (4)$$

where  $\Delta u_i$  is the difference between displacements on opposite sides of the unit cell specified by the difference position vector  $\Delta x_j$ . The strain components are specified as  $\bar{\epsilon}_{12} = \bar{\epsilon}_{21} = \gamma/2$  and  $\bar{\epsilon}_{11} = \bar{\epsilon}_{22} = 0$ , where  $\gamma$  is the applied

shear strain. The work-conjugate shear stress  $\tau$  is calculated as:

$$\tau = \frac{1}{2L^2} \int_C (T_1 x_2 + T_2 x_1) dC, \quad (5)$$

where  $T_i = \sigma_{ij} n_j$  is the traction on the boundary  $C$  of the unit cell with  $n_j$  the outward unit normal.

The doubly-periodic pure shear calculations were carried out on  $L = 10 \mu\text{m}$  unit cells for grain sizes  $d$  ranging from 0.2 to 5.0  $\mu\text{m}$ . The polycrystals were composed of two types of grains in an arrangement analogous to a checkerboard, where each grain differs in type from its four adjacent neighbors. Each grain has slip planes either at  $\phi = 0^\circ$  or  $\phi = 90^\circ$  with respect to the  $x_1$  axis. Resolving the dislocation dynamics requires a small time step of  $\Delta t = 0.5$  ns. The calculations were carried out with a rather high loading rate of  $\dot{\gamma} = 2000 \text{ s}^{-1}$  in order to reduce the CPU time required.

## 3. Numerical results

The predicted shear stress  $\tau$  versus applied shear strain  $\gamma$  curves for the LSD and HSD polycrystals are plotted in Fig. 1a and b for grain sizes in the range  $0.2 \mu\text{m} \leq d \leq 5 \mu\text{m}$ . Following an initial elastic response (since the crystals are elastically isotropic, the elastic response is uniform), a yield point characterized by a deviation from the elastic response is seen in all cases with the yield strength increasing with decreasing grain size  $d$  for both the LSD and HSD cases. The hardening behavior of the LSD and HSD polycrystals is markedly different. In the LSD case, the large grain polycrystals have a nearly ideally plastic response but the hardening rate increases sharply with decreasing grain size. In the HSD case, the large grain polycrystals have a mildly softening response with the smaller grained polycrystals exhibiting nearly ideally plastic behavior.

The shear flow strength,  $\bar{\tau}$ , defined as the average shear stress between  $\gamma = 0.15$  and 0.25%, is plotted in Fig. 2a for the LSD and HSD cases as a function of the grain size  $d$ . In both cases,  $\bar{\tau}$  increases with decreasing  $d$  with  $\bar{\tau}$  higher for the LSD case for any given grain size  $d$ . A relation of the form:

$$\bar{\tau} - \tau_0 = k \left( \frac{d}{d_0} \right)^{-n}, \quad (6)$$

is fit to the LSD and HSD data in Fig. 2a where  $\tau_0$  is the shear flow strength of a single crystal with only  $\phi = 0^\circ$  (or  $\phi = 90^\circ$ ) slip planes and  $d_0$  is a reference grain size taken to be 1  $\mu\text{m}$ . Such single crystal calculations revealed that  $\tau_0 \approx 25$  MPa for the LSD case and  $\approx 15$  MPa for the HSD case<sup>1</sup>. The best fit equations employing these values of  $\tau_0$  are indicated in Fig. 2a and reveal that the values for the Hall-Petch exponent,

<sup>1</sup> The lower strength of the HSD single crystal is attributed to the higher source density giving a greater number of low strength sources as a consequence of the Gaussian distribution of source strengths.

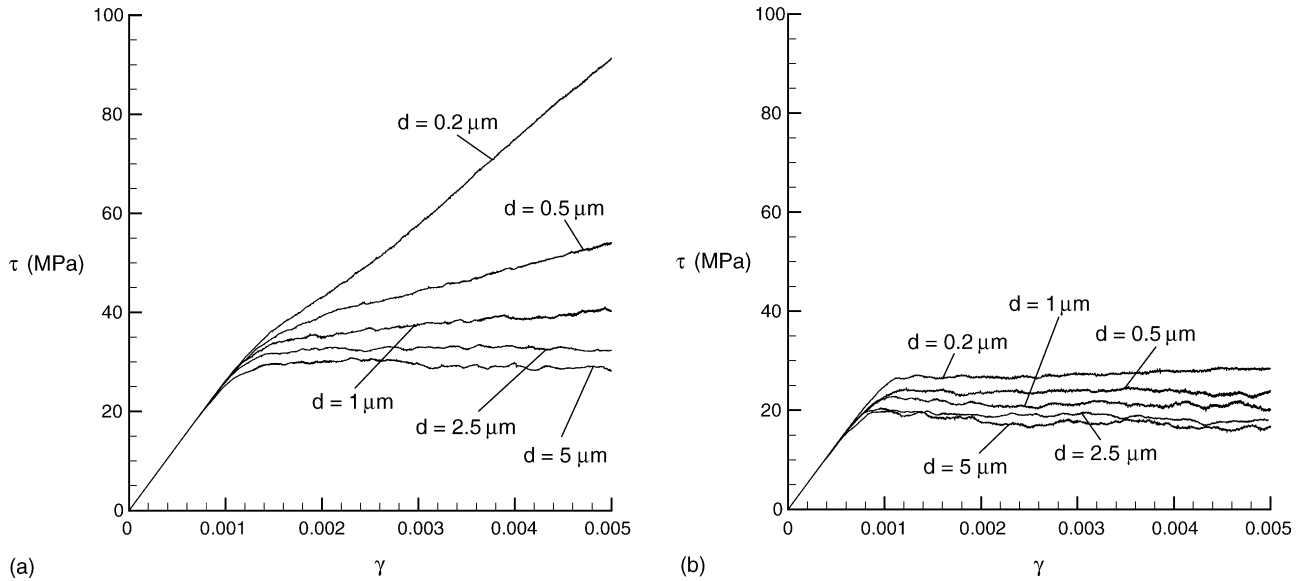


Fig. 1. Shear stress vs. shear strain for all grain sizes for (a) the LSD case and (b) the HSD case.

$n = 0.40$  and  $0.45$  in the LSD and HSD cases, respectively, are consistent with a wide body of experimental data.

The shear flow strength  $\bar{\tau}$  is plotted in Fig. 2b for the LSD and HSD cases as a function of the dislocation density averaged between  $\gamma = 0.15$  and  $0.25\%$ ,  $\bar{\rho}_{dis}$ . For a given source density,  $\bar{\rho}_{dis}$  increases with increasing  $\bar{\tau}$  indicating that the flow strength is consistent with a relation of the form of Eq. (2). We fit the relation:

$$\bar{\tau} - \tau_0 = c \left( \frac{\bar{\rho}_{dis}}{\rho_0} \right)^m, \quad (7)$$

to the LSD and HSD data in Fig. 2b with  $\tau_0$  set equal to the value of the single crystal flow strength and  $\rho_0$  a reference dislocation density taken to be  $1 \mu\text{m}^{-2}$ . These fits give power law exponents  $m = 1.03$  and  $0.76$  for the LSD and HSD cases rather than  $0.5$  as specified by (2).

Combining the fits in Eqs. (6) and (7) gives  $\bar{\rho}_{dis} \propto d^{-0.39}$  and  $\bar{\rho}_{dis} \propto d^{-0.59}$  in the LSD and HSD cases, respectively. Both the mean-free path model of Embury [6] and the plastic incompatibility model of Ashby [8] suggest that the dislocation density scales with  $d^{-1}$ . Thus, even though the discrete dislocation simulations predict a Hall-Petch exponent not far

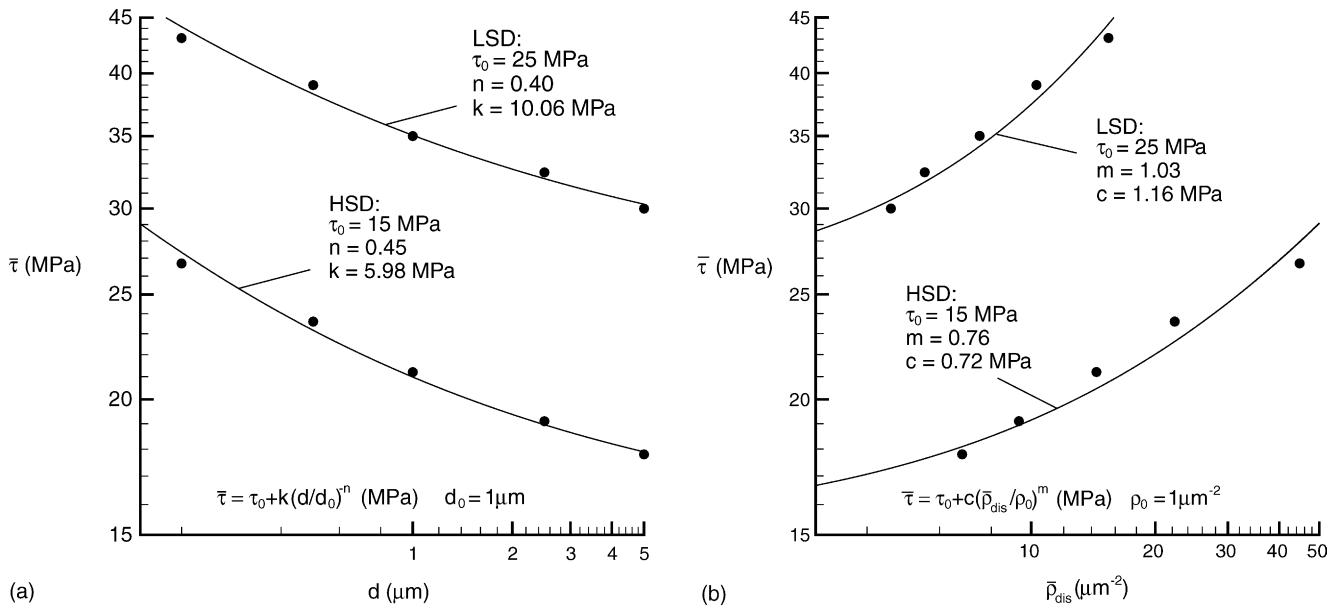


Fig. 2. Average shear stress between  $\gamma = 0.15$  and  $0.25\%$  for both the LSD and HSD cases plotted against (a) grain size, (b) average dislocation density between  $\gamma = 0.15$  and  $0.25\%$ . The solid lines give fits to the data.

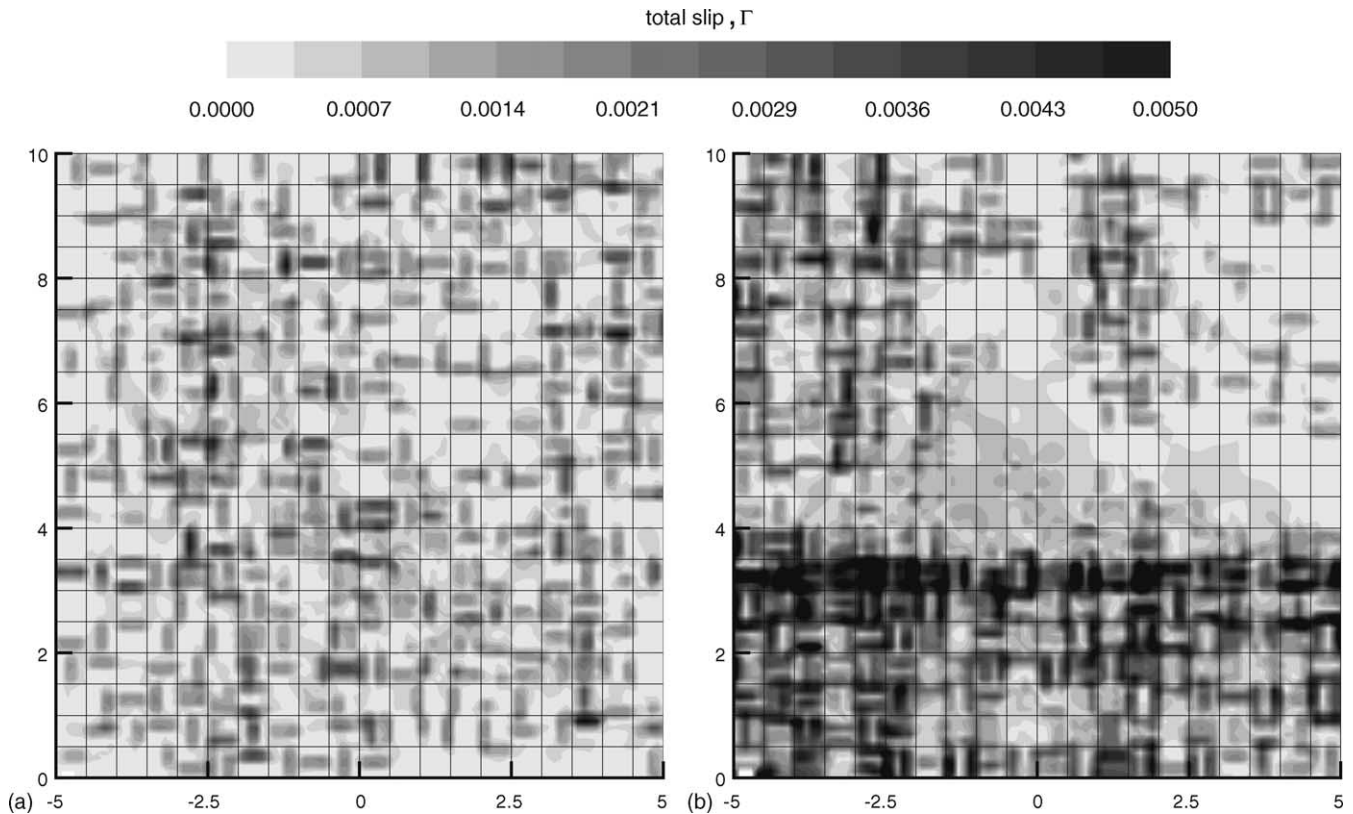


Fig. 3. Contours of total slip  $\Gamma$  for  $d = 0.5 \mu\text{m}$  for (a) the LSD case and (b) the HSD case at a shear strain  $\gamma = 0.2\%$ . The marked grid illustrates boundaries of the square grains over the unit cell.

from  $n = 0.5$ , the scaling of dislocation density with grain size does not fit these models.

For a given source density, the variation of flow strength with grain size is consistent with Eq. (2). However, for a given grain size,  $d$ , the dislocation density is lower for the LSD polycrystal than for the corresponding HSD polycrystal. Thus, when comparing polycrystals of the same grain size but of different source density, the behavior is opposite to that in Eq. (2). In order to understand this, we consider the distributions of plastic slip in the polycrystal. The calculation of the plastic slip involves averaging the displacement jumps across the slip planes. In particular, the values of the displacements  $u_i$  are evaluated on the finite element mesh and the strain field  $\epsilon_{ij}$  is obtained by numerical differentiation. Slip is then defined as  $\gamma^{(\alpha)} = s_i^{(\alpha)} \epsilon_{ij} m_j^{(\alpha)}$ , where  $s_i^{(\alpha)}$  is the tangent and  $m_j^{(\alpha)}$  is the normal to slip system  $\alpha$ . With single slip,  $\Gamma = |\gamma^{(\alpha)}|$  in each grain. Contours of  $\Gamma$  are plotted in Fig. 3a and b, for the  $d = 0.5 \mu\text{m}$  polycrystal for the LSD and HSD cases at a shear strain  $\gamma = 0.2\%$ . In the HSD case, a continuous slip band is seen to form across the entire unit cell resulting in a low yield strength with no hardening. However, in the LSD case plastic deformation is more diffused over the unit cell with no band of localized deformation visible. Thus, continued deformation is expected to result in the accumulation of geometrically necessary dislocations to accommodate the plastic incompatibility between adjacent grains,

giving rise to a higher yield strength and the hardening seen in Fig. 1a.

We find that the Hall-Petch relation and strain hardening behavior are sensitive to the initial dislocation source density. Over the range of source densities considered, both the flow strength and dislocation density increase with decreasing grain size. The predicted Hall-Petch exponents of  $n = 0.40$  and  $0.45$ , for the LSD and HSD cases, respectively, are consistent with a wide body of experimental data. Decreasing the initial source density prevents the formation of an easy slip path across the polycrystal which results in a higher flow strength and a higher hardening rate due to the accumulation of geometrically necessary dislocations associated with the plastic incompatibility between adjacent grains.

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