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DISCRETE DISLOCATION PLASTICITY ANALYSIS OF SIZE EFFECTS IN SINGLE CRYSTALS

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Summary. *The effect of size and slip system configuration on the tensile stress-strain response of micron-sized planar crystals as obtained from discrete dislocation plasticity simulations is presented. The crystals are oriented for either single or symmetric double slip. With the rotation of the tensile axis unconstrained, there is a strong size dependence, with the flow strength increasing with decreasing specimen size. Below a certain specimen size, the flow strength of the crystals is set by the nucleation strength of the initially present Frank-Read sources. The main features of the size dependence are the same for both the single and symmetric double slip configurations.*

1 INTRODUCTION

There is a considerable body of experimental evidence that plastic deformation in crystalline solids is size dependent at length scales of the order of tens of microns and smaller. This is typically associated with plastic strain gradients and geometrically necessary dislocations, see for example Ebeling and Ashby[1] and Fleck et al.[2]. However, there is growing evidence that plasticity size effects exist even when loading is compatible with an overall homogeneous deformation state as in the single crystal compression tests of of Uchic et al.[3] and Greer at al.[4]. In these experiments, cylinders, with diameters from $0.5\,\mu$m to $40\,\mu$m and height to diameter ratios in the range 2:1 to 4:1, were machined from a bulk single crystal using a focused ion beam microscope (FIB) and subject to uniaxial compression using a nanoindenter with a flat tip. While the Ni and Ni_3Al intermetallic crystals studied by Uchic et al.[3] were oriented for single slip, Greer et al.[4] employed gold single crystals mainly oriented in a symmetric double slip configuration. In these experiments, the flow strength of the smallest specimens was about an order of magnitude greater than that of the larger specimens but still substantially below the theoretical strength that would be expected to prevail for defect-free whiskers.

Two-dimensional discrete dislocation simulations of Deshpande et al.[5] have shown that the mechanism for the increasing strength with decreasing size in crystals oriented for single slip is largely consistent with the "dislocation starvation" picture of Greer et al.[4]. Here, we also present results from Deshpande et al.[6], using two-dimensional small-strain discrete dislocation plasticity to investigate the size dependent tensile response of crystals oriented for symmetric double slip.

2 DISCRETE DISLOCATION FORMULATION

We consider elastically isotropic crystals with Young's modulus $E = 70$ GPa and Poisson's ratio $\nu = 0.33$. Consistent with the plane strain assumption, only edge dislocations are considered, which have a Burgers vector $b = 0.25$ nm. The undeformed crystals are of dimension $2L \times W$ with $L/W = 1.5$ to match the aspect ratio in the experiments of Uchic et al.[3] and the specimen sizes varied from $W = 0.25\,\mu$m to $W = 8.0\,\mu$m. Initially, the crystal is free of mobile dislocations, but dislocations can generate from sources that are equally dispersed over the slip planes with a density of $\rho_{\rm src} = 56\,\mu{\rm m}^{-2}$. The sources nucleate a dipole when the Peach-Koehler force exceeds a critical value of $\tau_{\rm nuc} b$ over a period $t_{\rm nuc} = 10$ns; $\tau_{\rm nuc}$ is taken to have a Gaussian distribution with a mean strength $\bar{\tau}_{\rm nuc} = 50\,$MPa and a standard deviation of 1 MPa. There is also a random distribution of point obstacles with strength $\tau_{\rm obs} = 150\,$MPa and density $\rho_{\rm obs} = 56\,\mu{\rm m}^{-2}$. The drag coefficient for glide is $B = 10^{-4}\,$Pa s, which is a representative value for several FCC crystals. Here we present results for crystals oriented for symmetric double slip, that is the crystals have slip systems at $\phi = \pm 45°$ with the positive x_1 axis as sketched in Fig. 1. These results are contrasted with the predictions of Deshpande et al.[5] for crystals with one slip system at $\phi = 45°$ but otherwise identical to the ones analyzed here.

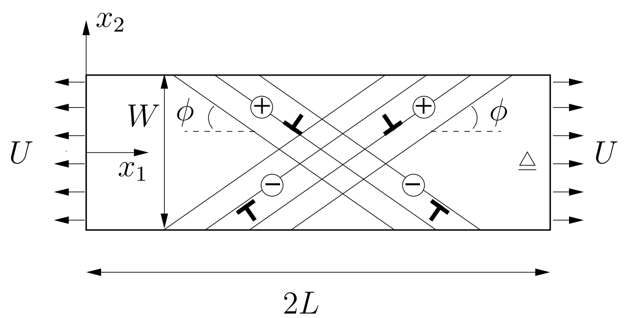

Figure 1: Sketch of the single crystal specimen analyzed and the sign convention employed for the edge dislocations.

The tensile axis of the specimen is aligned with the x_1 direction, see Fig. 1. Tension is imposed by prescribing $u_1 = U$, $T_2 = 0$ on $x_1 = 2L$ and $u_1 = -U$, $T_2 = 0$ on $x_1 = 0$, where $T_i = \sigma_{ij} n_j$ is the traction on the boundary with outward normal n_j. The lateral edges, on $x_2 = \pm W/2$, are traction free, i.e. $T_1 = T_2 = 0$. In addition, $u_2 = 0$ is imposed on one material point at $(2L - x_\epsilon, 0)$, where $x_\epsilon = 0.1L$. This prevents rigid body translation in the x_2 direction but does not restrict the rotation of the tensile axis of the specimen. Even though the rotation of the tensile axis of the specimen is unconstrained, the displacement boundary conditions, prevent the rotation of the ends of the specimen. This condition is representative of the constraints in the compression tests of Uchic et al.[3] and Greer et al.[4]. A time step of $\Delta t = 0.5\,\mathrm{ns}$ is needed to resolve the dislocation dynamics so a rather high loading rate $\dot{U}/L = 2000\,\mathrm{s}^{-1}$ is used to obtain a strain of 0.01 in $10,000$ time steps.

3 UNIAXIAL TENSION WITH SYMMETRIC DOUBLE SLIP

The tensile stress, σ, versus strain, U/L, responses of three specimen sizes of the crystals oriented for symmetric double slip are plotted in Fig. 2a. In all calculations in Fig. 2a, the first dislocation activity occurs at $\sigma \approx 95\,\mathrm{MPa}$. Since the Schmid factor for the slip system is $(\sin 2\phi)/2 = 0.5$, this value is consistent with the mean value of the source strength distribution being $\bar{\tau}_{\mathrm{nuc}} = 50\,\mathrm{MPa}$. Subsequently, for the $W = 1.0\,\mu\mathrm{m}$ and $4.0\,\mu\mathrm{m}$ specimens, there is a sharp drop in the stress followed by essentially an ideally plastic response. On the other hand, there is nearly no stress drop in the $W = 0.5\,\mu\mathrm{m}$ specimen with periodic fluctuations in the applied stress about a fixed mean value of the applied stress. These periodic fluctuations are associated with the nucleation and exit of dislocations from the $x_2 = \pm W/2$ traction-free boundaries. It is worth noting that in this specimen, the rate of dislocation nucleation is approximately equal to the rate at which dislocations exit the specimen.

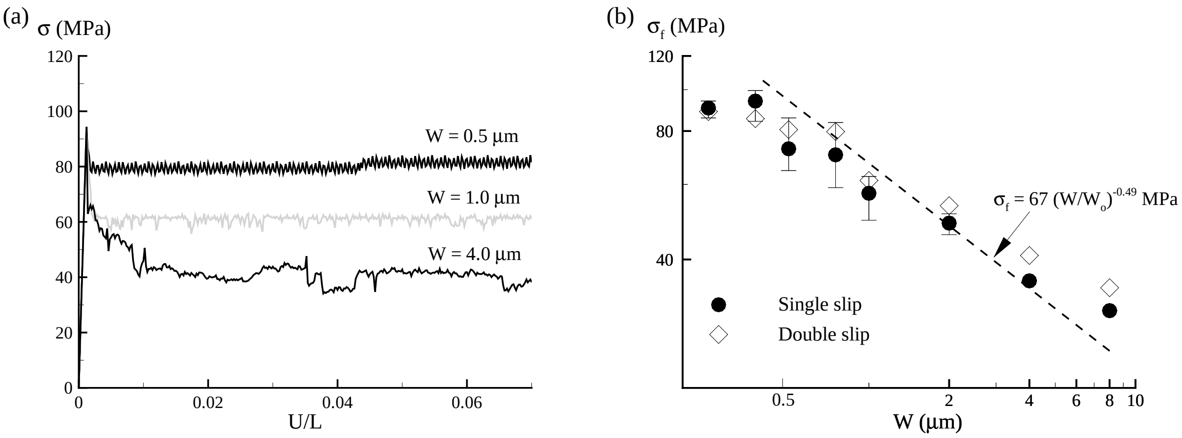

Figure 2: (a) Small-strain results for the tensile response of three sizes of single crystals oriented for symmetric double slip. (b) Flow strength σ_{f} as a function of the specimen size W for crystals oriented for single and symmetric double slip. Results from Deshpande et al.[5,6].

The results in Fig. 2a show that the flow strength is strongly dependent on the specimen size W. In order to quantify this size dependence, the flow strength σ_{f} (defined as the average stress between $0.04 \leq U/L \leq 0.05$) is plotted in Fig. 2b as a function of the specimen size W. The results indicate that the flow strength σ_f increases with decreasing W before leveling off at $W \approx 0.375\,\mu$m. Also included in Fig. 2b are the predictions of Deshpande et al.[5] for crystals with one slip system at $\phi = 45°$ (but otherwise identical to the symmetric double slip crystals analyzed here). The variation in flow strength with W in the single and symmetric double slip crystals is almost identical.

A power-law relation of the form

$$\sigma_\mathrm{f} = \alpha \left(\frac{W}{W_0} \right)^{-n}, \tag{1}$$

where $W_0 = 1\,\mu$m is a reference size, fits the data in Fig. 2b well over the range $0.75\,\mu\mathrm{m} \leq W \leq 4.0\,\mu$m with the choices $\alpha = 67\,$MPa and $n = 0.49$. Figure 2b indicates that while the flow strength scales approximately as $\sigma_\mathrm{f} \propto W^{-0.5}$ for intermediate sizes, there exist lower and upper plateaus of the flow strength with the large specimens ($W = 8.0\,\mu$m) having a flow strength higher than that given by eq. (1) while the small specimens ($W < 0.4\,\mu$m) have a flow strength less than that estimated from eq. (1). Since the flow strength of the small specimens is governed by the nucleation stress of the sources, $\sigma_\mathrm{f} \approx 2\bar{\tau}_\mathrm{nuc}/\sin 2\phi$ for $W < 0.4\,\mu$m.

In summary, the simulations suggest that the basic mechanisms of size dependence are similar in the single and symmetric double slip experiments of Uchic et al.[3] and Greer et al.[4] and consistent with the “dislocation starvation” picture[4].

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