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ABSTRACT: A deformation experiment has been developed specifically for the purpose of validation of dislocation dynamics simulations of plastic flow up to strains on the order of 1% [1]. The experiment has been designed so that a compressive uniaxial stress field is essentially super imposed on the test sample, and the crystal is free to deform with 3 orthogonal translation directions, and 3 rotation/tilt axes of freedom and has been given the name "6-degrees of freedom" (6DOF) experiment. The rotation, tilt and translation of the crystal are monitored by 5 laser displacement gages and 3 extensometers. Experiments are being performed on high purity Mo single crystals orientated for "single slip". All of the experiments are performed in pairs, with one test sample having highly polished surfaces for optical light and AFM slip-trace analyses, and the other having 4 strain gage rosettes mounted on the sides for measurement of the bi-axial surface strains during testing. All of the experimental data is used together to determine the slip activity of the orientated single crystal during deformation. Experimental results on high-purity Mo single crystals are presented. The results of these experiments show that slip behavior is in substantial deviation from the expected "Schmid" behavior. These experimental results bring into question some of the fundamental assumptions used in both the construction of crystal plasticity constitutive relationships and rules for dislocation mobility use in 3-D dislocation dynamics simulations.

INTRODUCTION: When a single crystal deforms, the various slip-system activities typically result in irregular shape changes. In deformation experiments, these irregular shape changes can lead to nonuniformities in stress states in the crystal and/or a nonuniform strain field. Because of this possibility, researchers must take special care to understand both the crystal's stress state and shape change during deformation if they wish to collect the information needed to validate 3-D DD-simulation results.

Our experimental technique was developed to minimize the nonuniformities in stress state that can occur during the deformation of single crystals. This technique was specifically developed to enable the validation of 3-D, discrete DD simulations. When using this technique, a deformation experiment is performed in compression; this allows essentially unconstrained deformation of single crystals that are oriented for a "single slip" under a condition of uniaxial stress. Several diagnostic techniques evaluate the crystal's shape change during deformation.

RESULTS AND CALCULATION OF SLIP SYSTEM ACTIVITY: The lower platen translation in the x and y directions during the axial deformation is shown in Figure 1. This plot indicates the relative motion of the center of the bottom of the test sample with respect to the center of the top in the laboratory reference frame. Slip trace ananlyses indicated that the $(10\bar{1})$, $(0\bar{1}\bar{1})$, and $(01\bar{1})$ slip planes were active.

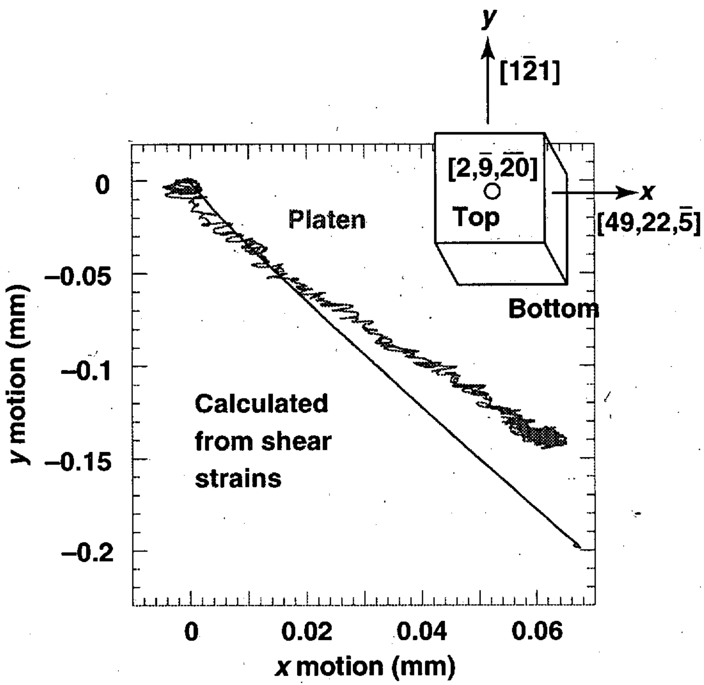

Figure 1. The translation of the bottom of the test sample as measured by the laser sensors. The calculated translation based on the strain gage measurements is in good agreement.

The approach used to calculate slip system activity follows the classical slip analysis that relates a general change in strain state to slip activity on five independent slip systems [3]. Our analysis focused on the six {110} slip planes, each of which have two <111> slip directions for a total of 12 possible slip systems. There are 384 possible combinations of five independent slip systems of the {110}<111> type that need to be considered. The symmetric Schmid orientation tensor associated with a single slip system, α, is given by

$$\mathbf{M}^{\alpha} = \frac{1}{2}\left(b^{\alpha} \otimes n^{\alpha} + n^{\alpha} \otimes b^{\alpha}\right), \tag{1}$$

where b^{α} is the slip direction defined by the Burgers vector and n^{α} is the slip plane normal related to the slip system α. Only one combination of the five independent slip systems (out of all 384 possible groups) matched the observed slip traces: slip systems 2, 4, 7, 8, and 10 (see Table I for crystallographic indices). The resolved-shear-stress versus shear-strain curves determined by our analysis for these systems is shown in Figure 2.

DISCUSSION: The $\left[2,\bar{9},\overline{20}\right]$ compression axis of the Mo single crystal test samples was selected to promote "single slip," with the primary slip system, $\left(\bar{1}01\right)\left[111\right]$, having a Schmid factor of 0.5. However, the observed deformation response was found to be inconsistent with "single slip" on this slip system. If the sole cause of deformation had been slip activity in the primary slip system, the displacement of the lower platen with respect to the upper platen would have been in the negative *x* direction, and there would not have been any displacement in the *y* axis. The observed displacement in the *x* direction was found to be opposite to this (i.e., positive x displacement), and the displacement in the y direction was substantially greater than the displacement in the x direction. The calculated slip system activity is in substantial deviation from the expected "Schmid" , i.e., the primary slip system is not the most active. Thus, the experimental results bring into question some of the fundamental assumptions used in both the construction of crystal plasticity constitutive relationships and rules for dislocation mobility use in 3-D dislocation dynamics simulations for bcc Mo.

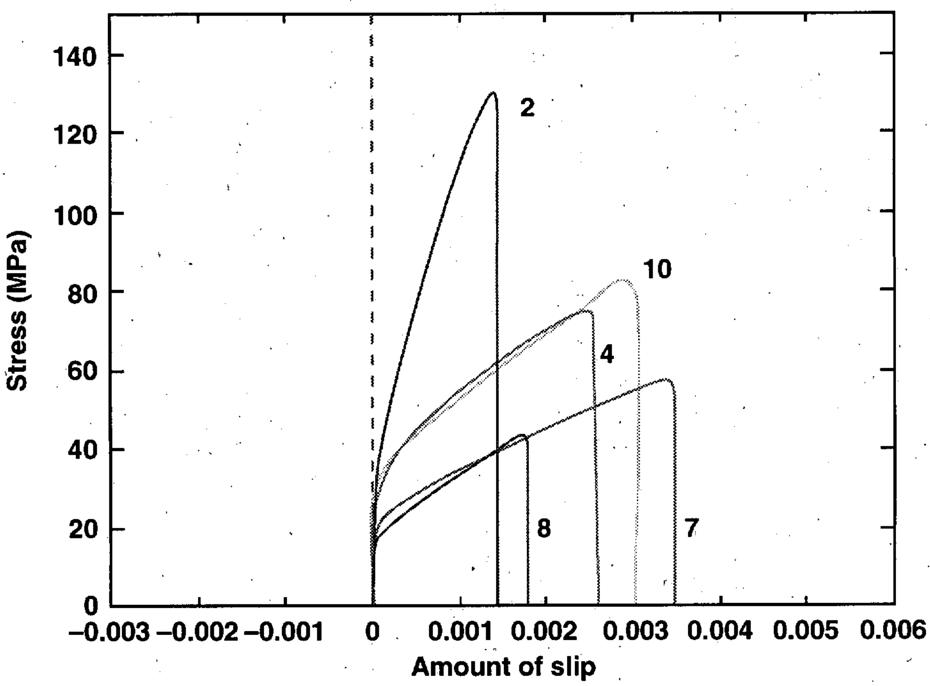

Figure 2. Plots of resolved-shear-stress versus shear-strain calculated from Eq. (5). The selected slip systems are 2, 4, 7, 8, and 10 (see Table for index notation).

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