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The statistical origin of bulk mechanical properties and slip behavior in fcc metals

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Abstract

A dislocations-based model is presented for predicting the flow stress of a pre-deformed metal single crystal. The model is based upon a combination of basic dislocation physics, the distribution of dislocation segment lengths in cell walls and percolation theory. With only the magnitude of the Burgers vector and the elastic shear modulus as inputs, and with no adjustable parameters, the model correctly predicts the formation of slip lines and slip bands, the linear behavior of the stress–strain curve in stage II hardening, the Voce behavior in stage III and the magnitude of the flow stress for deformed Al single crystals.

Keywords: Dislocations; Work hardening; Percolation

1. Introduction

In 1995, the late Dr. O. Richmond issued a challenge to the dislocations community [1]. He pointed out that no dislocations-based theoretical framework existed for predicting the flow stress of a pre-deformed metal single crystal. In this paper, we present such a framework. The model assumes that an underlying dislocation cellular structure exists (late stages II and III work hardening), that the Peierls stress is negligible and that the edge and screw mobilities are comparable. Thus, the model is most realistic for face centered cubic (fcc) metals. The only material parameters required by the model are the Burgers vectors, $\boldsymbol{b}$, and the elastic shear modulus, μ. The model correctly predicts the formation of slip lines and slip bands, the linear relationship between stress and strain during stage II work hardening, the Voce relationship during stage III and the magnitude of the flow stress for deformed single crystal Al. This paper concentrates on a physical description of the model and its predictions; the full mathematical details and derivations will be published elsewhere.

2. Description of the model

Fig. 1 shows an atomic force microscope (AFM) image of the surface of an Al single crystal [2]. The crystal was deformed 15% in uniaxial tension along a $\langle 2\,5\,28\rangle$ axis to develop a dislocation cellular structure, then electropolished to remove the existing slip lines and slip bands, and finally deformed an additional 4% in situ in the AFM. The pronounced surface steps are slip bands that are composed of many individual slip lines. Deformation is spatially heterogeneous and occurs through the nucleation and growth of these bands.

Transmission electron microscope studies were conducted on an identical tensile specimen deformed 15% along the same axis [3]. The average cell size is much smaller than the lengths of the slip bands shown in Fig. 1. Thus, the dislocations that travel through the bulk to form slip lines on the sample surface must traverse many dislocation cells and remain roughly on a single slip plane. This behavior demonstrates that slip events originate from a single nucleation site and propagate through many dislocation cells.

In our model, the nucleation and propagation of slip events result from the unstable bowing of pinned dislocation line segments in the cell walls (for instance from dislocation junctions). Thus, if the stress is raised on an unloaded sample that

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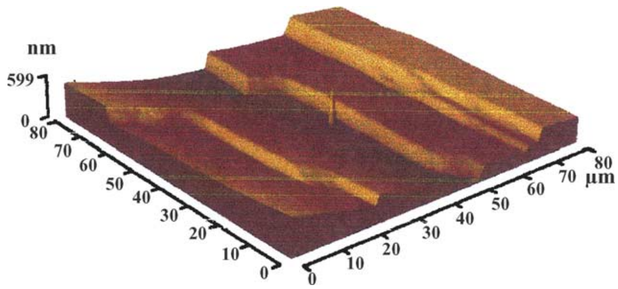

Fig. 1. AFM image of plastically deformed Al single crystal.

possesses a mature dislocation cellular structure, dislocation segments in the walls will progressively bow-out until the longest unblocked segment in the gauge section becomes unstable, traverses a dislocation cell and produces an increased localized stress on the adjacent cell walls. The critical bow-out stress is given approximately by $\sigma_c = \mu \boldsymbol{b}/l$ where l is the segment length. The expression for σ_c is the average bow-out stress for edge and screw dislocations [4]. Depending upon the distribution of dislocation segment lengths in these adjacent walls and the new total stress, additional dislocations may then bow-out, producing a dislocation cascade that can propagate across the entire sample. Thus, the nucleation and propagation of a slip event both depend crucially upon the size distribution of pinned dislocation segments in the sample.

As mentioned previously, the dislocation cell walls develop during stage II work hardening. Since stage II is temperature independent, relaxation processes can be neglected and the segment length distribution function (SLDF) may be approximated by a random distribution of pinning points on dislocations of total length L, where L is the average dislocation cell size. A derivation that is only rigorous for large numbers of pinning points indicated that the functional form for the resulting SLDF is

$$P(l) = \frac{1}{\bar{l}}\left(1 - \frac{l}{L}\right)^{N_0-1}, \tag{1}$$

where P is the probability of finding a segment of length l, N_0 the number of pinning points on the dislocation and $\bar{l}$ is the average segment length. Computer simulations in which small numbers of random pinning points were added to dislocation lines were conducted and the resulting SLDF was indistinguishable from Eq. (1). Since the SLDF develops during deformation, any dislocation segments longer than the critical bow-out length at the maximum applied stress would already have bowed out. Thus, the correct distribution function has a cutoff at large l as shown in Fig. 2.

If a dislocation loop is incident upon a cell wall, the added stress field is quite localized and only interacts significantly with a small fraction of the dislocations in the wall. We characterize this interaction volume by a scalar, n_L, that represents the number of "unblocked" dislocations that interact significantly with the incident dislocation. Using this definition and with the SLDF from Eq. (1) as a starting point, it was possible

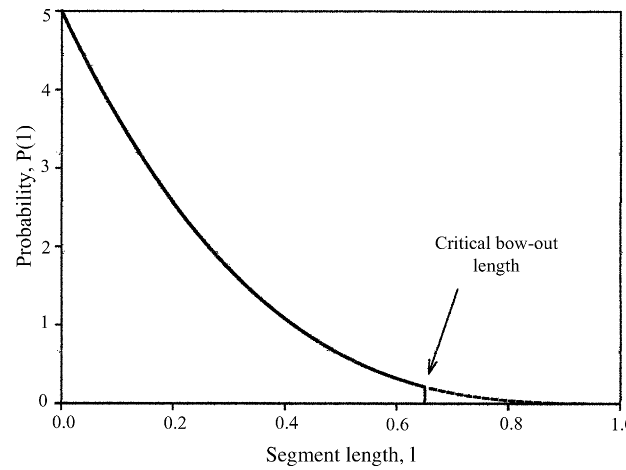

Fig. 2. Segment length distribution function for stage II with $L = 1$ and $N_0 = 4$. The critical bow-out length was chosen for visual clarity.

to derive an analytical expression for the probability, P_T of s^* dislocations being emitted from the opposite side of a wall with s incident dislocations and a macroscopic applied stress of σ_a

$$P_T(s^*) = P_1^{s^*}(1 - P_1)^{n_L - s^*}\frac{n_L!}{s^*!(n_L - s^*)!},$$
$$P_1 = 1 - \left(1 - \left(1 - \frac{l_{FR}}{L}\right)^{N_0}\right)^{N_0+1},$$
$$l_{FR} = \frac{\mu \boldsymbol{b}}{\sigma_a(s+1)} \tag{2}$$

where $\sigma_a(s+1)$ is the local stress on a wall with s dislocations piled up against it.

The dislocation transmission function given by Eq. (2) was used to program percolation simulations similar to those published previously using more empirical transmission functions [5–7]. The cellular structure was assumed to have a square geometry with a fixed cell size. Since the number of primary dislocations in the interaction volume of the cell walls is expected to be small, a Poisson distribution for n_L was assumed in the simulations. The statistical internal state variables for the model are therefore N_0, $\langle n_L \rangle$ and L. Fig. 3 shows the resulting critical surface for pure Al with a 2 µm dislocation cell size. The only other inputs were the magnitude of the Burgers vector and the elastic shear modulus. The ranges chosen for N_0 and $\langle n_L \rangle$ are "educated guesses" based upon TEM data from deformed single crystal Al samples. The vertical axis is a direct prediction of the flow stress (projected onto the primary slip plane) and the magnitude agrees well with our own flow stress measurements from Al single crystals during tensile deformation.

The detailed behavior of the model can be determined by tracking the trajectory of a point in the parameter space shown in Fig. 3. For this virtual experiment, we will use an infinitely stiff, displacement controlled testing machine. Since L changes very slowly with strain, we will assume for this discussion that L is a constant. Starting at a point below the