Plasticity of BCC metals from atomic scale to continuum

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Body-centered cubic (BCC) metals are crystallographically simple materials whose plastic deformation is nevertheless governed by processes that are not common in face-centered cubic (FCC) metals. These differences are rooted at the atomic level, where the cores of $1/2\langle 111\rangle$ screw dislocations in BCC metals are inherently nonplanar [1], which contrasts the plane cores of dissociated $1/2\langle 110\rangle$ dislocations in FCC crystals. Due to the nonplanar spreading of the former dislocations, their motion is not affected only by the shear stress in the $\{110\}$ slip plane acting parallel to the slip direction (i.e., the Schmid stress) but, in principle, by all components of the stress tensor [2]. Under small strains and strain rates relevant for engineering applications, the critical resolved shear stress (CRSS) acting in the maximum resolved shear stress plane (MRSSP) parallel to the slip direction was shown [2,3] to depend on: (i) the angle χ of the MRSSP, and (ii) the magnitude of the shear stress perpendicular to the slip direction. This information was obtained by molecular statics simulations on isolated screw dislocations [4] using Bond Order Potentials (BOP) [5] and predicts the occurrence of anomalous slip in BCC Mo and W that has been observed experimentally in all nonmagnetic BCC metals. We have represented the obtained atomistic data mathematically using a relatively simple yield criterion, $\tau_0 + \sum_{i=1}^{3} a_i \tau_i = \tau_{cr}^*$ that depends linearly on two shear stresses parallel and two perpendicular to the slip direction, both acting in two different $\{110\}$ planes in the zone of the slip direction. The four adjustable parameters (a_1, a_2, a_3, τ_{cr}^*) are obtained by fitting the results of atomistic simulations. We will utilize this criterion to predict the activity of twelve $\{110\}\langle 111\rangle$ systems in BCC Mo and W under tension and compression. It suggests the existence of tension-compression asymmetry, which has been observed in the past five decades in all BCC metals. The parametrization sometimes requires further fine-tuning using experimental data as evidenced by comparing theoretical predictions with recent in situ experiments on compressed micropillars [6].

The link between the atomistic studies of isolated screw dislocations and macroscopic response of the material is established by formulating a thermodynamic model of thermally activated slip that is based on the Arrhenius law $\dot{\gamma} = \dot{\gamma}_0 \exp[-\Delta H(\tau)/kT]$. Here, $\Delta H(\tau)$ is the activation enthalpy needed to transform a straight screw dislocation at the applied stress τ into the curved configuration that needs no additional energy to surmount the periodically varying lattice friction and thus to move through the crystal. This stress dependence of the activation enthalpy can be obtained from a model derived using the variational calculus [7]. The most important inputs into this model are the Peierls barrier, its variation with the applied stress, and the curvature of the dislocation pathway, all of which can be obtained using Nudged Elastic Band (NEB) calculations on a straight dislocation [8]. We will highlight the underlying assumptions in these models and propose ways to include further details such as the orientational dependence of the dislocation line energy and interactions between dislocation segments in the activated state. This thermodynamic model will be used to predict the temperature dependence of the flow stress and compare it with experimental measurements [9,10]. This methodology is applicable not only to all nonmagnetic BCC metals but also to ferromagnetic α-Fe whose plastic deformation is simplified by the lack of anomalous slip.

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