ANALYTICAL PLASTIC FLOW RULES FOR BCC METALS INVOLVING NON-SCHMID EFFECTS

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ABSTRACT We have performed atomistic simulations of an isolated screw dislocation in bcc Mo and W using Bond Order Potentials [Gröger, 2007]. Based on these results we formulated an effective yield criterion that reproduces the non-Schmid behavior of dislocations in these materials. This yield criterion was subsequently used to develop a mesoscopic theory of thermally activated plastic flow that involves the effects of both the temperature and the plastic strain rate. In this paper, we unify these results into continuum-level plastic flow rules that will be used in the future in large-scale dislocation dynamics simulations.

INTRODUCTION Plastic flow of bcc metals is governed by motion of $1/2\langle 111\rangle$ screw dislocations that posses non-planar cores spread on the three $\{110\}$ planes in the zone of the $\langle 111\rangle$ slip direction. Due to this spreading, the Peierls stress of screw dislocations is generally a function of both the orientation of the plane in which the shear stress parallel to the Burgers vector that drives the dislocation glide is applied, the so-called maximum resolved shear stress plane (MRSSP), and of the magnitude of the shear stress perpendicular to the slip direction. These dependencies were calculated using semi-empirical Bond Order Potentials for Mo and W [Gröger, 2007] and used subsequently to formulate effective yield criteria for these metals. Based on these results, we constructed two-dimensional Peierls potential that is then used to calculate the activation enthalpy using a two-dimensional version of the Dorn and Rajnak [1964] model of nucleation of kink pairs. The calculated temperature dependencies of the yield stress for Mo and W agree with a number of deformation experiments in both tension and compression. In this paper, we unify these results into continuum-level plastic flow rules and show that the calculated temperature and strain rate dependence of the yield stress agrees well with experimental measurements.

ANALYTICAL PLASTIC FLOW RULES In its most general form, the effective yield criterion for bcc metals is written as a linear combination of four terms:

$$\tau^{*\alpha} = \mathbf{m}^\alpha \mathbf{\Sigma}^c \mathbf{n}^\alpha + a_1 \mathbf{m}^\alpha \mathbf{\Sigma}^c \mathbf{n}_1^\alpha + a_2(\mathbf{n}^\alpha \times \mathbf{m}^\alpha)\mathbf{\Sigma}^c \mathbf{n}^\alpha + a_3(\mathbf{n}_1^\alpha \times \mathbf{m}^\alpha)\mathbf{\Sigma}^c \mathbf{n}_1^\alpha \leq \tau^*_{cr} \ , \quad (1)$$

where α designates a particular $\{110\}\langle 111\rangle$ slip system, $\mathbf{m}^\alpha$ is the slip direction, $\mathbf{n}^\alpha$ the slip plane normal, $\mathbf{n}_1^\alpha$ the normal of the so-called non-glide plane that makes angle $60°$ with the slip plane, and a_1,a_2,a_3,τ^*_{cr} are adjustable parameters determined by fitting the results of atomistic simulations. The first two terms in $\tau^{*\alpha}$ reproduce the dependence on shear stresses parallel to Burgers vector, while the last two capture the effect of the shear stress perpendicular to the slip direction. In (1), the applied loading is expressed as the stress tensor $\mathbf{\Sigma}^c$, and $\tau^*_{cr} - \tau^{*\alpha}$ is thus a measure of the "distance" from the yield surface.

Hence, yielding on the slip system α occurs when $\tau^{*\alpha}$ reaches τ^*_{cr}. The yield criterion (1) was employed to develop a mesoscopic theory of thermally activated plastic flow in bcc metals that involves both the temperature and the plastic strain rate. This theory predicts the temperature dependence of the yield stress or, equivalently, the dependence of the plastic strain rate $\dot{\gamma}^\alpha/\dot{\gamma}_0$ on the effective stress $\tau^{*\alpha}/\tau^*_{cr}$, where $\dot{\gamma}_0$ is a pre-exponential factor in the Arrhenius law assuming that the mobile dislocation density is a constant. The approximation of this dependence becomes more intuitive when written in the logarithmic form, where $\ln(\dot{\gamma}^\alpha/\dot{\gamma}_0)$ behaves asymptotically at negative $\ln(\tau^{*\alpha}/\tau^*_{cr})$ and becomes zero as $\ln(\tau^{*\alpha}/\tau^*_{cr}) \to 0$, i.e. when $\tau^{*\alpha}$ reaches τ^*_{cr}. Therefore, $\dot{\gamma}^\alpha$ can be approximated as

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \exp\left\{-\frac{A}{kT}\left[B - \tanh\left(C\left(\ln\frac{\tau^{*\alpha}}{\tau^*_{cr}} + D\right)\right)\right]\right\} \ , \tag{2}$$

where k is the Boltzmann constant and A, B, C, D parameters that are to be determined by fitting the $\ln(\dot{\gamma}^\alpha/\dot{\gamma}_0) - \ln(\tau^{*\alpha}/\tau^*_{cr})$ data calculated from the proposed theory of thermally activated plastic flow. At zero stress, i.e. when $\tau^{*\alpha} \to 0$, the tanh in (2) yields -1 and the rate equation reduces to $\dot{\gamma}^\alpha = \dot{\gamma}_0 \exp(-2H_k/kT)$, where $2H_k = A(B+1)$ is the energy of two isolated kinks on a straight screw dislocation. At large stresses approaching the Peierls stress, i.e. when $\tau^{*\alpha} \to \tau^*_{cr}$, the activation enthalpy vanishes and the rate equation has to read $\dot{\gamma}^\alpha = \dot{\gamma}_0$, which implies that the argument of the exponential in (2) is $A[B - \tanh(CD)] = 0$. The four unknown parameters A, B, C, D can now be determined by adjusting A and C that control the height and slope of the tanh function in (2), after which B and D are obtained from the two conditions above.

In the case of simple loading such as uniaxial loading, it is possible to invert (2) to obtain an analytical dependence of the yield stress (or τ^*_{cr}) on temperature and strain rate. For each slip system α characterized by the slip plane normal $\mathbf{n}^\alpha$ and the slip direction $\mathbf{m}^\alpha$, one can identify the MRSSP in the zone of the slip direction in which the shear stress parallel to the slip direction is at maximum. The orientation of this MRSSP relative to the $\{110\}$ slip plane of system α is denoted as χ^α and the uniaxial stress is resolved in this plane as a combination of the shear stresses parallel (σ^α) and perpendicular (τ^α) to the slip direction. Hence, the four matrix terms in (1) can be written using the parameters χ^α and $\eta^\alpha = \tau^\alpha/\sigma^\alpha$ and the τ^* criterion reduces to $\tau^{*\alpha} = \sigma^\alpha t(\chi^\alpha, \eta^\alpha) \le \tau^*_{cr}$. In this expression, $t(\chi^\alpha, \eta^\alpha) = \cos\chi^\alpha + a_1\cos(\chi^\alpha + \pi/3) + \eta^\alpha[a_2 \sin 2\chi^\alpha + a_3\cos(2\chi^\alpha + \pi/6)]$. At yield, σ^α reaches the yield stress σ^α_{cr} and $\tau^{*\alpha} = \sigma^\alpha_{cr} t(\chi^\alpha, \eta^\alpha)$. This equation can be substituted in (2) to arrive at the temperature and strain rate dependence of the yield stress for system α:

$$\sigma^\alpha_{cr} = \frac{\tau^*_{cr}}{t(\chi^\alpha, \eta^\alpha)} \exp\left\{-D + \frac{1}{C}\tanh^{-1}\left[B + \frac{kT}{A}\ln\frac{\dot{\gamma}^\alpha}{\dot{\gamma}_0}\right]\right\} \ . \tag{3}$$

Here, a_1, a_2, a_3, τ^*_{cr}, A, B, C, D are the material's constants that are determined as outlined above.

COMPARISON WITH EXPERIMENTS In order to compare the predictions of the analytical expression (3) with experiments, we consider uniaxial loading of Mo in tension along the $[\bar{1}49]$ axis for which Hollang et al. [1997] measured the temperature dependence of the yield stress. For this orientation, the $(\bar{1}01)[111]$ system (α) is activated for slip first and the MRSSP corresponding to the $[111]$ slip direction coincides with the $(\bar{1}01)$ plane, i.e.

$\chi^\alpha = 0$. The ratio of the two shear stresses resolved in this MRSSP is $\eta^\alpha = 0.51$. For a given experimental plastic strain rate, we determine $\dot{\gamma}_0$ from the requirement that the activation enthalpy at the temperature T_k where the thermal component of the yield stress vanishes is equal to the energy of two isolated kinks, $2H_k = 1.27$ eV. The τ^* criterion for Mo is characterized by parameters $a_1 = 0.24$, $a_2 \approx 0$, $a_3 = 0.35$ and $\tau^*_{cr} = 1014$ MPa, obtained from atomistic calculations, and the constants $A = 0.9$, $B = 0.41$, $C = 0.6$, $D = 0.73$.

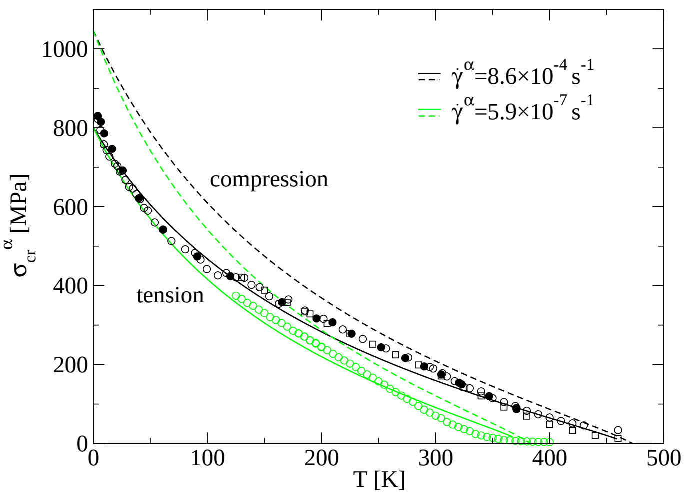

Figure 1: Temperature dependence of the yield stress for Mo calculated from (3) (curves) and measured in tension by Hollang et al. [1997] (symbols). The yield stress σ^α_{cr} is resolved in the $(\bar{1}01)$ plane.

In Fig. 1 we compare the temperature dependence of the yield stress for loading in tension obtained from (3) (solid curves) with the measurements of Hollang et al. [1997] (symbols). For both experimental plastic strain rates $\dot{\gamma}$, the simple equation (3) reproduces correctly the overall temperature dependence of the yield stress. In the region of temperatures where the plastic flow is thermally activated, the yield stress to move the dislocation increases with decreasing temperature. As $T \to 0$, the yield stress rises to its maximum and the stress to move a single dislocation becomes equal to the Peierls stress. On the other hand, at high temperatures, the yield stress vanishes and the plastic flow becomes athermal. For comparison, we also plot in Fig. 1 the dependencies predicted for loading in compression along $[\bar{1}49]$. Clearly, for this orientation, the yield stress in compression is higher than that in tension which is in agreement with the experiments of Seeger and Hollang [2000]. However, for loading axes close to the $[011] - [\bar{1}11]$ edge of the stereographic triangle, the character of this asymmetry changes and the yield stress in tension becomes higher than that in compression. This result is again in agreement with the measurements of Seeger and Hollang [2000]. For details, refer to Gröger [2007] available online as `arXiv:0707.3577`.

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