Effect of Non-Glide Stresses on Deformation of BCC Metals at Finite Temperatures

Roman Gröger and Vaclav Vitek

Department of Materials Science and Engineering, University of Pennsylvania, 3231 Walnut Street, Philadelphia, PA 19104-6272, U.S.A.

ABSTRACT

In this paper, we show that plastic flow of bcc metals at finite temperatures and strain rates can be captured by a model in which the underlying physics enters via the results of single-dislocation atomistic studies at 0 K. The Peierls potential is constructed solely from the results of atomic-level calculations and accounts for both the crystal symmetry and the effect of non-glide stresses. This potential is then employed in calculations of the stress dependence of the enthalpy to nucleate a pair of kinks, which is used subsequently to evaluate the temperature and strain rate dependence of the yield stress. Results of these calculations are shown to be in excellent agreement with experimental data.

1. Introduction

The plastic deformation of all bcc metals is controlled by $1/2\langle 111\rangle$ screw dislocations that have non-planar cores and, therefore, possess a very high Peierls stress. This leads to a strong temperature dependence of the flow stress at low temperatures. In addition, the non-planar core also induces a pronounced tension-compression asymmetry [1] that has commonly been interpreted in terms of the twinning-antitwinning asymmetry of the sense of shearing in the slip direction. However, detailed atomistic calculations [2, 3] have disclosed that the situation is more complex and that the Peierls stress is also a strong function of the shear stress perpendicular to the slip direction. These studies, which employed molecular statics and thus correspond to 0 K, have ascertained the dependence of the critical resolved shear stress (CRSS) for glide, i.e. the Peierls stress, of the 1/2[111] screw dislocation as a function of: (i) the angle χ between the maximum resolved shear stress plane (MRSSP) and the $(\bar{1}01)$ plane and (ii) the shear stress τ perpendicular to the slip direction. These results have then been utilized to construct an effective yield criterion that correctly captures the effect of non-glide stresses [3, 4]. When formulating such criterion we define an effective stress τ^* as a linear combination of shear stresses parallel and perpendicular to the slip direction in two different {110} planes:

$$\tau^* = \sigma\left[\cos\chi + a_1\cos(\chi+\pi/3)\right] + \tau\left[a_2\sin 2\chi + a_3\cos(2\chi+\pi/6)\right]. \qquad (1)$$

Here σ is the shear stress parallel to the slip direction acting in the MRSSP and the yield criterion is then $\tau^* \le \tau^*_{cr}$ where τ^*_{cr} is an effective yield stress. a_1, a_2, a_3 and τ^*_{cr} are parameters determined by fitting the $\mathrm{CRSS}-\chi$ and $\mathrm{CRSS}-\tau$ dependencies obtained from atomistic calculations. In the case of molybdenum, $a_1 = 0.24$, $a_2 = 0$, $a_3 = 0.35$, $\tau^*_{cr}/C_{44} = 0.027$.

At finite temperatures, a moving dislocation surmounts the Peierls barrier at stresses lower than the Peierls stress via the formation of pairs of kinks and with the aid of thermal activation. However, 0 K calculations do not determine the Peierls barrier but merely its maximum slope along a transition coordinate ξ defined as the minimum-energy path between two adjacent equivalent potential minima. The Peierls stress σ_P and the Peierls barrier $V(\xi)$ are related by

$$\sigma_P b = \max\left(dV/d\xi\right). \qquad (2)$$

For a given angle χ of the MRSSP and angle ψ, which the slip plane makes with the $(\bar{1}01)$ plane, the Peierls stress can be expressed as $\sigma_P = \mathrm{CRSS}\cos(\chi - \psi)$. Since screw dislocations do not have well-defined slip planes, it is necessary to consider a two-dimensional Peierls potential, $V(x, y)$, defined in the plane perpendicular to the dislocation line. The height and shape of this potential and, most importantly, its dependence on the applied stress tensor, are crucial information for the development of a theory of the thermally activated motion of screw dislocations.

In this paper, we first show how the Peierls potential and its dependence on the stress tensor can be extracted from the data obtained in atomistic studies at 0 K. Using this information we then develop a model of the formation of pairs of kinks following the approach of Dorn and Rajnak [5]. We then employ this model in the analysis of the temperature and orientation dependence of the yield stress in molybdenum the results of which are compared with experimental observations [6-8]. In the following, the yield stress is always expressed as the shear stress parallel to the slip direction resolved in the $(\bar{1}01)$ plane.

2. Construction of the Peierls potential

The shape of the effective Peierls potential, $V(x, y)$, is based on a mapping function, $m(x, y)$, that is defined in the plane perpendicular to the dislocation line, i.e. (111) plane in the case of the 1/2[111] screw dislocation. This function captures periodicities and symmetries in this plane, in particular the symmetry-dictated positions of potential minima, maxima and saddle points. It is shown in Fig. 1 as a contour plot where dark regions are potential minima and bright regions potential maxima; the maximum height of $m(x, y)$ is one.

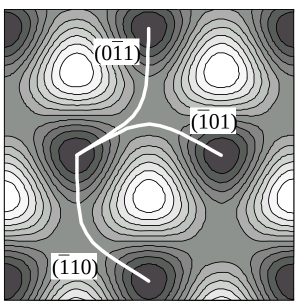
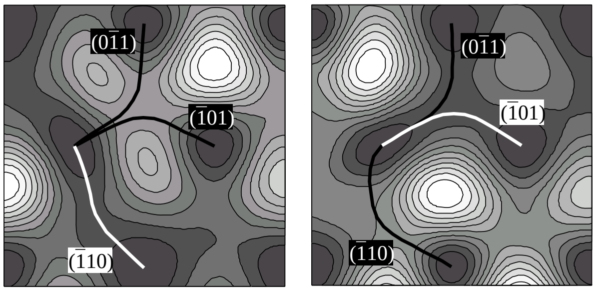


Figure 1: Mapping function m(x,y). The white curves depict the three equivalent minimum energy paths between the potential minima.

We begin the construction of the effective Peierls potential by capturing the fundamental symmetries in the (111) plane. This can be accomplished by writing $V(x, y) = \Delta V\, m(x, y)$, where ΔV is a currently unknown potential height. To determine ΔV, we investigate loading by pure shear, σ, parallel to the slip direction for χ=0. For this loading, atomistic studies show that the dislocation moves along the $(\bar{1}01)$ plane, i.e. ψ=0, and thus $\sigma_P = \mathrm{CRSS}$ in (2). The shape of the Peierls barrier, $V(\xi)$, experienced by the dislocation is obtained as a cross-section of $V(x, y)$ along the transition coordinate ξ defined above that, in the present case, connects two adjacent potential minima on the $(\bar{1}01)$ slip plane. This minimum-energy path has been determined numerically using the Nudged Elastic Band method. The potential height, ΔV, is then obtained to satisfy (2).

In order to incorporate the effect of non-glide stresses, we first generalize the Peierls potential within each repeat cell of the (111) plane to $V(x, y) = [\Delta V + V_\sigma(\theta)]\, m(x, y)$, where θ is a polar angle in the (111) plane measured in the same sense as χ and ψ, and the term $V_\sigma(\theta)$ represents an angular distortion of the three-fold symmetric basis of the potential by the non-glide stress σ applied in a plane *different* than $(\bar{1}01)$. The functional form of the added term is written as $V_\sigma(\theta) = K_\sigma(\chi)\, \sigma b^2 \cos\theta$ which obeys the symmetry of the shear stress parallel to the slip direction and assures that the largest distortion is always applied in the $(\bar{1}01)$ plane. In this equation, the function $K_\sigma(\chi)$ is determined from the requirement that (2) reproduces the $\mathrm{CRSS} - \chi$ dependence obtained from atomistic studies. Since in these calculations the glide is always along the $(\bar{1}01)$ plane and thus ψ=0 for any orientation of the MRSSP, the Peierls stress in (2) becomes $\sigma_P = \mathrm{CRSS}\cos\chi$ and the corresponding value of $K_\sigma(\chi)$ can be found by numerically solving (2) when ΔV has already been fixed.

Finally, the effect of the shear stress perpendicular to the slip direction, τ, is incorporated by writing $V(x,y) = [\Delta V + V_\sigma(\theta) + V_\tau(\theta)]\, m(x,y)$, where $V_\tau(\theta)$ represents an angular distortion of the Peierls potential by τ. The functional form of $V_\tau(\theta)$ is now chosen such that it reproduces the symmetry of the shear stress perpendicular to the slip direction and, simultaneously, is a linear function of τ. One of the simplest forms that satisfies both these requirements is $V_\tau(\theta) = K_\tau(\chi)\, \tau b^2 \cos\left(2\theta + \pi/3\right)$. In order to keep the evaluation of $K_\tau(\chi)$ relatively simple, we consider $\chi \in \left(-\pi/6, +\pi/6\right)$ and shear stresses $\tau / C_{44} = \pm 0.01$ for which the dislocation glides on the $(\bar{1}01)$ plane. The Peierls stress in (2) is thus again $\sigma_P = \mathrm{CRSS} \cos\chi$ and the values of $K_\tau(\chi)$ for a given χ can be found by numerically solving (2). Very importantly, the Peierls potential has been constructed only from the data corresponding to the $(\bar{1}01)$ slip and the change of the slip plane at large negative τ, observed in atomistic studies, is not included *a priori*. The contour plots of the distorted Peierls potential for two different values of τ and $\chi = 0$ are shown in Fig. 2.



a) τ/C_{44}=-0.05 b) τ/C_{44}=+0.05

Figure 2: Effect of the shear stress perpendicular to the slip direction, τ, on the shape of the effective Peierls potential V(x,y). The curves define the minimum energy paths for the dislocation glide along the three different {110} planes. The white path has the lowest Peierls barrier.

The effective Peierls potential, $V(x,y)$, developed as described above, reproduces correctly both the twinning-antitwinning asymmetry of the shear stress parallel to the slip direction and the effect of the shear stress perpendicular to the slip direction. It is seen from Fig. 2b that for positive τ the Peierls potential displays a low-energy path along the most-highly stressed $(\bar{1}01)$ plane, which thus leads to a low Peierls barrier for slip on this plane. However, this slip is suppressed at negative τ (Fig. 2a) where the lowest Peierls barrier corresponds to the glide along the $(\bar{1}10)$ plane. For other orientations of the MRSSP and negative τ, the low-energy path typically develops either on the $(\bar{1}10)$ or on the $(0\bar{1}1)$ plane. The Schmid stress in these planes is much lower than in the $(\bar{1}01)$ plane and the slip can thus be classified as anomalous. This finding is in excellent agreement not only with 0 K atomistic studies [2, 3] but also with experiments [6]. Interestingly, since the possibility of slip on other planes than $(\bar{1}01)$ has not been assumed in the construction of the Peierls potential, the anomalous slip at negative τ follows *naturally* from the chosen shape of the term $V_\tau(\theta)$.

3. Activation enthalpy and the temperature dependence of the yield stress

At stresses lower than the Peierls stress, the dislocation moves towards the top of the Peierls barrier and, simultaneously, the originally three-fold symmetric basis of the Peierls potential gets distorted by the action of σ and τ. The activation enthalpy ΔH for nucleation of a pair of kinks, which depends on the shape of the Peierls potential, can be evaluated using the model of Dorn and Rajnak [5]. The plastic strain rate $\dot{\gamma}$ is then given by the standard relation of the reaction rate theory

$$\dot{\gamma} = \dot{\gamma}_0 \sum_\alpha \exp[-\Delta H^\alpha(\sigma,\tau)/kT]. \qquad (3)$$

where ΔH^α is the stress-dependent activation enthalpy for the slip system α. When considering only the most operative slip system with the lowest ΔH and setting $\dot{\gamma}_0$ to comply with an effective density of mobile dislocations, the temperature dependence of the yield stress can be obtained for a given strain rate from the relation $\Delta H(\sigma,\tau) = kT \ln(\dot{\gamma}_0/\dot{\gamma})$.

The symbols in Fig. 3 show the temperature dependence of the yield stress measured by Hollang *et al* [7] for single crystals of Mo under loading in tension along $[\bar{1}49]$ and two plastic strain rates. Since this loading leads to the single slip on the $(\bar{1}01)[111]$ system, the temperature dependence of the yield stress can be readily calculated and it is depicted in Fig. 3 by solid lines. At stresses lower than 115 MPa, the slip occurs by nucleating two interacting kinks and the activation enthalpy is determined by the elastic interaction of kinks [9] (dashed lines in Fig. 3). An excellent agreement between the theory and experiments is obvious.

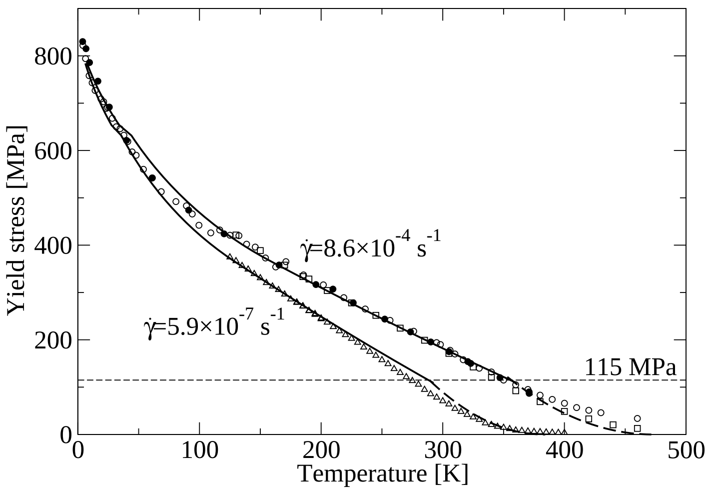


Figure 3: Temperature dependence of the yield stress for tension along $[\bar{1}49]$. The experimental data are from [7].

For loading along $[\bar{1}49]$ the MRSSP is the $(\bar{1}01)$ plane (χ=0) and no twinning-antitwinning asymmetry is present. However, the calculated yield stress in compression is higher than in tension. This significant tension-compression asymmetry, caused by the shear stress perpendicular to the slip direction, is in good qualitative agreement with experimental observations [8]. Interestingly, if the loading axis deviates toward the [011] corner of the stereographic triangle, the tension-compression asymmetry changes its character and the yield stress in tension becomes larger than that in compression. This trend is again in agreement with the experiments in [8].

4. Conclusion

This paper shows how the results of single-dislocation atomistic studies at 0 K can be used to develop a mesoscopic theory of thermally activated dislocation motion and to finally attain the theoretical description of the temperature, strain rate and orientation dependence of the yield stress. This multiscale sequential combination of atomistic modeling with the dislocation theory results in the physically based multislip yield criteria for plastic flow of bcc metals at finite temperatures and strain rates.

References

1. J. W. Christian, *Metall. Trans. A, 14* (1983) 1237.
2. K. Ito and V. Vitek, *Philos. Mag. A, 81* (2001) 1387.
3. R. Gröger and V. Vitek, *Materials Science Forum, 482* (2005) 123.
4. V. Vitek, M. Mrovec and J. L. Bassani, *Mat. Sci. Eng. A, 365* (2004) 31.
5. J. E. Dorn and S. Rajnak, *Trans. TMS-AIME, 230* (1964) 1052.
6. P. J. Jeffcoat, B. L. Mordike and K. D. Rogausch, *Philos. Mag., 34* (1976) 583.
7. L. Hollang, M. Hommel and A. Seeger, *Phys. Stat. Sol. (a), 160* (1997) 329.
8. L. Hollang and A. Seeger, *Materials Transactions, JIM, 40* (2000) 141.
9. A. Seeger, *J Phys IV, 5* (1995) 45.