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Complex macroscopic plastic flow arising from non-planar dislocation core structures

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Abstract

For a broad range of crystalline materials complex dislocation core structures have a significant effect on macroscopic plastic flow, causing unexpected deformation modes that are strongly influenced by other components of stress in addition to the glide stress on a given slip system and on the sign of stress. In this paper we use atomistic simulations of a screw dislocation in bcc molybdenum to determine the dependence on orientation of the maximum resolved shear stress (in the direction of the Burgers vector) required to move the dislocation. A yield criterion that enters a continuum theory of bcc crystal plasticity and includes non-glide components of stress is developed along the lines of a general framework that was proposed several years ago. The predicted results are in excellent agreement with the atomistic simulations. © 2001 Elsevier Science B.V. All rights reserved.

Keywords: Dislocation core structures; Non-glide stresses; bcc yield criteria; Macroscopic plastic flow; Slip system

1. Introduction

Ample evidence now exists for a broad range of crystalline materials, particularly those with non-close-packed lattices, that dislocation core structures have a significant influence on macroscopic plastic flow (for recent reviews see [1–5]). Common signatures of core effects are: unexpected deformation modes and slip geometries; strong and unusual dependence of flow stresses on crystal orientation and temperature; and, most commonly, a break-down of Schmid's law which states that glide on a given slip system, defined by a slip plane and direction of slip, commences when the resolved shear stress on that system, the Schmid stress, reaches a critical value. Implicitly other components of the stress tensor and, for well-annealed crystals, the sign of stress are assumed to play no role in the deformation process. Schmid's law was established originally for metals with close-packed crystal structures [6]. These assumptions are often invalid for materials in which the dislocation core effects are important (see, for example, [2,7–11]). This was emphasized prominently by Sir Alan Cottrell in the closing address of a conference to celebrate the '50th Anniversary of the Concept of Dislocations in Crystals,' [12]: '... for too long we have taken the fcc dislocation as the paradigm of all dislocation behavior; but, as the studies of bcc screw dislocations have shown, the fcc structures and properties are the exception rather than the norm.'

At the same time the overwhelming majority of studies of plastically deforming crystals made in the framework of the finite-strain continuum theory [13–16] have assumed the Schmid-type constitutive behavior. Consequently, these studies principally apply to fcc metals in which plastic deformation is, indeed, controlled by the shear stress acting on a slip plane in the slip direction. In fcc metals the dissociation of dislocations into Shockley partials keeps them confined to the close-packed {111} planes for every orientation of the dislocation line and, therefore, they possess planar core structures and obey Schmid's law. On the other hand, in materials with more complex and open structures the cores may spread into several non-parallel planes for some orientations of the dislocation line.

In this paper we focus on the break down of the Schmid law due to non-planar cores with the aim to incorporate these effects into the constitutive relations

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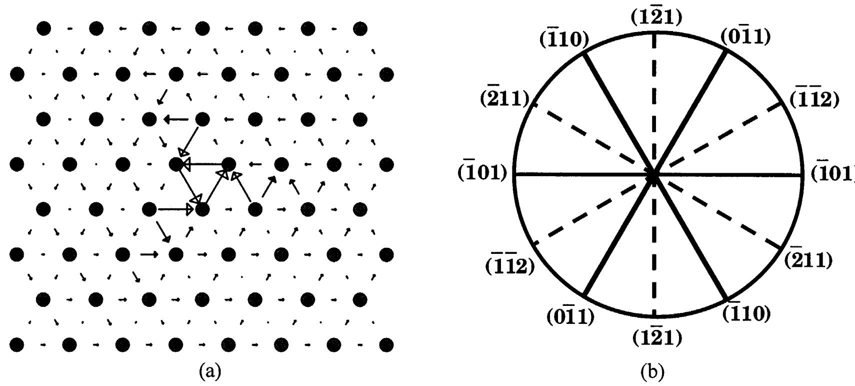

Fig. 1. (a) Structure of the core of the 1/2[111] screw dislocation depicted using differential displacements; (b) Orientations of all the {110} and {112} planes belonging to the [111] zone.

for macroscopic continuum models of plastically deforming crystals. Specifically, we concentrate on the slip behavior arising from the non-planar spreading of the 1/2⟨111⟩ screw dislocation in bcc metals that is generally regarded as controlling many important features of slip in these materials [5,17]. Two distinct deviations from Schmid's law can be identified. First, the critical resolved shear stress (CRSS) for slip may depend on the shear stress in the slip direction acting in different planes of the core spreading that could be alternative slip planes. Secondly, the CRSS may be influenced by other components of the applied stress tensor, in particular shear stresses in the direction perpendicular to the Burgers vector. In the case of the screw dislocation in bcc metals this can be attributed to small edge components of displacement within the core of screw dislocations [8,9,11,18].

In the present study we concentrate only on the effect of shear stresses in the slip direction acting on planes into which the core spreads. In the case of the 1/2⟨111⟩ screw dislocation these are three {110} planes of the ⟨111⟩ zone.[1] The dependence of the CRSS on the orientation of the maximum resolved shear stress plane is first studied by atomistic modeling of the glide of the 1/2⟨111⟩ screw dislocation. This dependence demonstrates the break-down of Schmid's law arising from the effect of shear stresses acting in the three {110} planes that contain the [111] direction and comprises the well-known twinning–anti-twinning asymmetry of slip observed in bcc metals [1,10,17]. Using a continuum framework for the effects of non-glide stresses [24,25] that was employed earlier in the case of Ni_3Al [16,26], we then construct the yield criterion that can accurately reproduce the stress-state dependence of the atomistic simulations. This criterion captures the slip characteristics arising from the atomic structure and properties of dislocation cores and thus provides a bridge between atomic and continuum scales in the study of the plastic deformation of bcc metals.

2. Atomistic study of the glide of 1/2[111] screw dislocations

The atomistic calculations presented in this paper have all been made using a many-body central force potential of the Finnis–Sinclair type for molybdenum [27] with a molecular statics relaxation method. The calculated core structure of the 1/2[111] screw dislocation is shown in Fig. 1a using the method of differential displacements [2].[2] To facilitate the interpretation of this picture the orientations of all the {110} and {112} planes belonging to the [111] zone are shown in Fig. 1b. It is seen that the core is spread principally into three {110} planes of the [111] zone. Since the core structure shown in Fig. 1a is not invariant with respect to the [10$\bar{1}$] diad, a symmetry operation of the bcc lattice, then another energetically equivalent configuration related by this symmetry operation must exist, as first pointed out in [22]. In this alternative configuration spreading of the core into three {110} planes is found on the other side relative to the line of their intersection. The

[1] Core structure of this type was first suggested on crystallographic grounds [19] and specific details of core spreading were then revealed by atomistic calculations of various sophistication (see, for example, [2,10,11,20,21]) though the main features were captured already in the early studies, the results of which were presented in Asilonar at ICSMA 2 [22]. Very recently this type of core spreading was confirmed experimentally in a high-resolution electron microscopic study of dislocations in molybdenum [23].

[2] The atomic arrangement is shown in the projection perpendicular to the direction of the dislocation line ([111]) and circles represent atoms within one period. The [111] component of the relative displacement of the neighboring atoms produced by the dislocation is depicted as an arrow between them. The length of the arrows is proportional to the magnitude of the relative displacements, and in this projection it is taken to be equal to the separation of neighboring atoms when the magnitude of the displacement is equal to |1/6[111]|.

core structure of the same type has been found in earlier calculations employing generic pair potentials [1,10,20,22], as well as in the recent calculations using quantum mechanics based non-central potentials [21].

The glide of the 1/2[111] screw dislocation arising from a shear stress parallel to the Burgers vector but not necessarily on the slip plane is studied in this paper for various planes corresponding to the maximum resolved shear stress plane (MRSSP). More general cases of stress application in tension and compression will be reported elsewhere [28]. The orientation of the MRSSP is defined by the angle χ which it makes with the $(\bar{1}01)$ slip plane as depicted in Fig. 2 and commonly used in earlier theoretical and experimental studies [1,17]. Due to the crystal symmetry it is sufficient to consider $-30° \leq \chi \leq 30°$. However, it should be noted that orientations corresponding $+\chi$ and $-\chi$ are not equivalent. In general, for an orientation χ the shear in the [111] direction is equivalent to the shear in the $[\bar{1}\bar{1}\bar{1}]$ direction for the orientation $-\chi$. But for a given χ shears along [111] and $[\bar{1}\bar{1}\bar{1}]$ are not generally equivalent because the (111) plane is not a mirror plane in the bcc lattice.[3] This asymmetry related to the sense of shearing has usually been described in terms of the twinning–anti-twinning asymmetry of shear on {112} planes but it applies to all planes of the ⟨111⟩ zone except {110} planes. Since the notion of the twinning–anti-twinning asymmetry is a common terminology (see, for example, [1,10,17,20]), we shall refer to the orientations of the MRSSP corresponding to $-30° \leq \chi \leq 0°$ orientations as those of twinning shear and $0° \leq \chi \leq 30°$ orientations as those of anti-twinning shear. When the sign of the applied stress changes the twinning and anti-twinning orientations interchange.

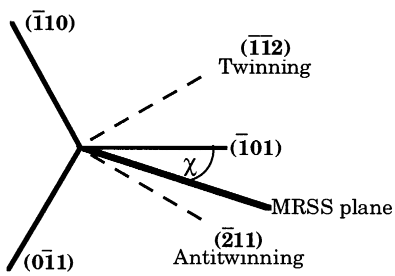

Fig. 2. Definition of the orientation of MRSSP described by the angle χ.

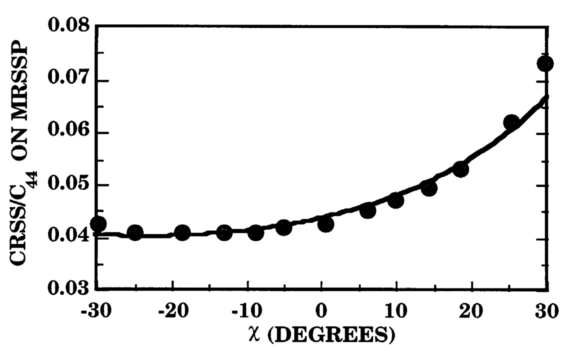

Fig. 3. Dependence of the CRSS (τ_M), normalized by the shear modulus C_{44}, on χ. Circles represent results of atomistic calculation and the curve corresponds to (Eq. (4)).

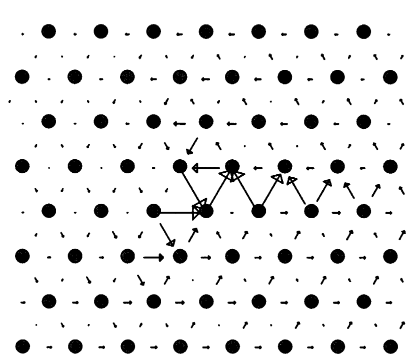

Fig. 4. Structure of the core of the 1/2[111] screw dislocation for the resolved shear stress of $0.04C_{44}$ with the MRSSP corresponding to $\chi = 30°$ i.e. $(\bar{2}11)$ plane.

For a given orientation of the MRSSP the applied stress was imposed via the corresponding elastic displacement field evaluated using anisotropic elasticity. Starting with the fully relaxed core, the applied stress was increased incrementally and full relaxation carried out at every step until the dislocation started to move for that orientation. At that point, the applied shear stress, i.e. the MRSSP, is referred to as the CRSS (and as τ_M in Section 3). The calculated dependence of the CRSS on χ is shown in Fig. 3 for molybdenum. The dislocation moved along the $(\bar{1}01)$ plane for all values of χ except 30° when it moved on average along the $(\bar{2}11)$ plane but composed of equal segments of $(\bar{1}01)$ and $(\bar{1}10)$ planes. However, it should be noted that for $\chi = -30°$ the $(0\bar{1}1)$ and $(\bar{1}01)$ planes are equivalent.

Since the dependence of CRSS on χ does not follow $1/\cos\chi$, Schmid's law is not valid (for Schmid's law $\tau_M \cos\chi =$ critical value when the slip is on $(\bar{1}01)$). This can be attributed to the fact that prior to the dislocation motion the core changes under the influence of the applied stress and these changes are dependent on the orientation of the MRSSP, i.e. on the applied stress state. An example is shown in Fig. 4 where the displacement map of the dislocation core is shown for the case of $\chi = 30°$ for the resolved shear stress of $0.04C_{44}$, where C_{44} is the shear modulus. The spreading into the $(\bar{1}10)$ plane is constricted while spreading into the $(\bar{1}01)$ is extended; spreading into the $(0\bar{1}1)$ plane is practically unaffected. This suggests that these changes in the core are driven by the shear stresses in the corresponding {110} planes. In this case these stresses are the same for $(\bar{1}01)$ and $(\bar{1}10)$ planes while no shear stress acts on the

[3] These two shears are equivalent if the plane of shearing is of the {110} type owing to the ⟨110⟩ diad symmetry operation.

$(0\bar{1}1)$ plane. Hence, when constructing the yield criterion for continuum studies we can assume that it will be a function of the shear stresses on all three {110} planes of the [111] zone that will emulate the CRSS vs χ dependence found by atomistic calculations.

3. Yield criterion

To include the effects of non-glide components of stress in a single crystal yield criterion, Qin and Bassani [24] proposed that slip system α is at yield when a generalization of Schmid's law holds:

$$\tau^{*\alpha} = \tau^{\alpha} + \sum_{\eta} a_{\eta}^{\alpha}\tau_{\eta}^{\alpha} = \tau_{\rm cr}^{*\alpha}, \quad (1)$$

where τ^{α} is the Schmid stress and τ_{η}^{α} are the non-glide stresses associated with the slip system α, a_{η}^{α} are the material parameters that determine the relative importance of the different non-glide components, and $\tau_{\rm cr}^{*\alpha}$ is the critical value of the effective stress, for that system; the non-glide stresses τ_{η}^{α} are homogeneous functions of degree one in the stress tensor σ and summation is over the total number of non-glide components. The effective stress $\tau^{*\alpha}$ defines the yield function, and here for simplicity is taken to be linear in the stress. If $\tau^{*\alpha} = \tau^{\alpha}$, the Schmid stress, then (Eq. (1)) reduces to Schmid's law. In general, $\tau^{*\alpha}$ can be distinct from the (work conjugate) Schmid stress and will depend on many aspects of the crystal structure including the dislocation core structure. The yield criterion (Eq. (1)) for slip system α can be expressed as

$$\boldsymbol{\sigma}:\mathbf{d}^{*\alpha} = \tau_{\rm cr}^{*\alpha} \qquad \text{with } \mathbf{d}^{*\alpha} = \mathbf{d}^{\alpha} + \sum_{\eta} a_{\eta}^{\alpha}\mathbf{d}_{\eta}^{\alpha}, \quad (2)$$

where $\mathbf{d}_{\eta}^{\alpha}$ are the symmetric second-order slip system tensors that determine all relevant non-glide components ($\mathbf{d}^{\alpha}$ resolves the Schmid stress) and $\boldsymbol{\sigma}$: $\mathbf{d}\equiv\mathrm{tr}(\boldsymbol{\sigma}\cdot\mathbf{d}) = \sigma_{ij}d_{ij}$ In many cases, for example for cross-slip in fcc metals, slip in $L1_2$ intermetallic compounds, as well as in the present study of bcc metals, the non-glide stresses τ_{η}^{α} are also shear stresses, and then $\mathbf{d}_{\eta}^{\alpha}$ can be expressed in dyadic form

$$\mathbf{d}_{\eta}^{\alpha} = \frac{1}{2}(\mathbf{m}_{\eta}^{\alpha}\otimes\mathbf{n}_{\eta}^{\alpha} + \mathbf{n}_{\eta}^{\alpha}\otimes\mathbf{m}_{\eta}^{\alpha}), \quad (3)$$

where $\mathbf{m}_{\eta}^{\alpha}$ and $\mathbf{n}_{\eta}^{\alpha}$ can be regarded as lattice vectors on the same footing as the usual slip-system vectors which define the Schmid stresses; note that in this case $\mathbf{m}_{\eta}^{\alpha}$ $\mathbf{n}_{\eta}^{\alpha} = 0$.

For the case of dislocations in bcc lattices which is the focus of this paper, we are motivated to consider the shear stress acting on other planes containing the Burgers vector for the reasons discussed above. Because we are only interested in a single slip system, the index α in the previous equations can be omitted from here on. First we note that all shear stresses in the direction of the Burgers vector can be written as a linear combination of the Schmid stress τ (on the $(\bar{1}01)$ plane of Fig. 2) and any other shear stress parallel to that vector, for example the shear stress on the $(0\bar{1}1)$ plane, $\tau_{(0\bar{1}1)}$. In the following we will introduce this non-glide-stress component into the yield criterion, writing (Eq. (1)) as

$$\tau + a\tau_{(0\bar{1}1)} = \tau_{\rm M}[\cos(\chi) + a\cos(\chi + 60)] = \tau_{\rm cr}^{*\alpha}, \quad (4)$$

where, as noted above,$\tau_{\rm M}$ denotes the CRSS on the MRSSP. As an example, for molybdenum we have chosen the two parameters, $\tau_{\rm cr}^{*}$ and a (the non-glide-stress coefficient), in this yield criterion from a least-square fit of the data in Fig. 3. The results are $\tau_{\rm cr}^{*}/C_{44} = 0.0586$ and $a = 0.641$. With these values the $\tau_{\rm M}$ vs. χ given by equation (Eq. (4)) is also plotted in Fig. 3 as a continuous curve. There is excellent agreement with the atomistic simulations.

It is expedient to note that with $\tau_{(\bar{1}10)}$ chosen as the non-glide-stress component, the value of $\tau_{\rm cr}^{*}$ is on the order of the applied stress, which seems reasonable. As mentioned above, we could consider the stress on any other plane containing the Burgers vector and the yield function would not change, but the values of the parameters $\tau_{\rm cr}^{*}$ and a would change. In particular, when the non-glide-stress was calculated on either the twinning or anti-twinning planes, the value of $\tau_{\rm cr}^{*}$ was not of the same order as $\tau_{\rm M}$. Although we have only reported results here for molybdenum, similar agreement was found in the case of tantalum.

4. Conclusions

We have utilized atomistic simulations of dislocation behavior to begin to develop a physically-based continuum theory of bcc crystal plasticity that incorporates the effects of non-glide components of the shear stress. Further studies are underway to explore more general loading and the effects of shear stresses perpendicular to the Burgers vector. These results will be embedded in a full, three-dimensional continuum theory of multiple slip in bcc crystals in order to model the range of complex phenomena that are cited in the introduction and in a number of review papers on bcc plasticity.

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References

[1] M.S. Duesbery, in: F.R.N. Nabarro (Ed.), Dislocations in Solids, vol. 8, Elsevier Science Publ. BV, Amsterdam, 1989, p. 67.
[2] V. Vitek, Prog. Mater. Sci. 36 (1992) 1.
[3] F. Louchet, J. Phys. IV 3 (1993) 567.
[4] S. Takeuchi, Radiat. Eff. Defect Solid 148 (1999) 333.
[5] J.P. Hirth, Acta Mater. 48 (2000) 93.
[6] E. Schmid, W. Boas, Kristallplastizität, Springer, Berlin, 1928.
[7] Z.S. Basinski, M.S. Duesbery, in: R.C. Gifkins (Ed.), Proc. Sixth Int. Conf. on Strength of Metals andAlloys, Pergamon Press, New York, 1983, p. 21.
[8] M.S. Duesbery, Proc. Roy. Soc. London A 392 (1984) 145.
[9] M.S. Duesbery, Proc. Roy. Soc. London A 392 (1984) 175.
[10] V. Vitek, M.S. Duesbery, in: M. Meshii (ed.), Mechanical Properties of DCC Metals, TMS, Warrendale, PA, 1982, p. 3.
[11] M.S. Duesbery, V. Vitek, Acta Mater. 46 (1998) 1481.
[12] M.H. Lorretto, in: M.H. Lorretto (ed.), Dislocations and Properties of Real Materials, The Institute of Metals, London, 1985.
[13] J.R. Rice, J. Mech. Phys. Sol. 19 (1971) 433.
[14] R. Hill, J.R. Rice, J. Mech. Phys. Sol. 20 (1972) 401.
[15] R.J. Asaro, Adv. Appl. Mech. 23 (1983) 1.
[16] J.L. Bassani, Adv. Appl. Mech. 30 (1994) 191.
[17] J.W. Christian, Metall. Trans. A 14 (1983) 1237.
[18] K. Ito, V. Vitek, in: V. Bulatov, T.D. de la Rubia, R. Phillips, E. Kaxiras, N. Ghoniem (Eds.), Multiscale Modelling of Materials, vol. 538, Materials Research Society, Pittsburgh, 1999, p. 87.
[19] P.B. Hirsch, in: Proc. 5th Int. Conf. Crystallography, Cambridge University, 1960, p. 139.
[20] V. Vitek, Crystal lattice defects 5 (1975) 1.
[21] W. Xu, J.A. Moriarty, Moriarty, Phys. Rev. B 54 (1996) 6941.
[22] V. Vitek, in: W.C. Leslie (ed.), Second Int. Conference on the Strength of Metals and Alloys, ASM, Metals Park, Ohio, 1970, p. 389.
[23] W. Sigle, Philos. Mag. A 79 (1999) 1009.
[24] Q. Qin, J.L. Bassani, J. Mech. Phys. Sol. 40 (1992) 813.
[25] Q. Qin, J.L. Bassani, J. Mech. Phys. Sol. 40 (1992) 835.
[26] V. Vitek, D.P. Pope, J.L. Bassani, in: F.R.N. Nabarro, M.S. Duesbery (Eds.), Dislocations in Solids, vol. 10, Elsevier Science Publ. BV, Amsterdam, 1996, p. 135.
[27] G.J. Ackland, R. Thetford, Philos. Mag. A 56 (1987) 15.
[28] K. Ito, V. Vitek, 2000, to be published