Abstract

By direct application of stress in molecular statics calculations we identify the stress components that affect the glide of 1/2⟨111⟩ screw dislocations in bcc tungsten. These results prove that the hydrostatic stress and the normal stress parallel to the dislocation line do not play any role in the dislocation glide. Therefore, the Peierls stress of the dislocation cannot depend directly on the remaining two normal stresses that are perpendicular to the dislocation, as proposed by Koester A, Ma A, Hartmaier A. Acta Mater 2012;60:3894 but, instead, on their combination that causes an equibiaxial tension-compression (and thus shear) in the plane perpendicular to the dislocation line. The Peierls stress of 1/2⟨111⟩ screw dislocations then depends only on the orientation of the plane in which the shear stress parallel to the Burgers vector is applied and on the magnitude and orientation of the shear stress perpendicular to the slip direction.

Keywords: Peierls stress, Screw dislocation, Bcc metal, Non-glide stress, Yield criterion.

1. Introduction

It is generally accepted that the plastic deformation of body-centered cubic (bcc) metals is very different from that of close-packed crystals \( \{111\} \). The main reason is that the former is governed by the glide of 1/2⟨111⟩ screw dislocations whose cores are non-planar \( \{2 \overline{1} \langle 1 \rangle \} \). Consequently, the glide of these dislocations may be affected by all components of the applied stress tensor \( \{4\} \). These can be divided into two groups. The first are the stress components that contribute to the Peach-Koehler force on the dislocation and thus directly cause its glide. The remaining stress components do not exert any Peach-Koehler force on the dislocation, but they affect the slip by modifying the structure of the dislocation core.

Atomistic simulations made in Ref. \( \{4\} \) have shown that the Peierls stress of the 1/2⟨111⟩ screw dislocation in bcc metals depends on the orientation of the corresponding maximum resolved shear stress plane (MRSSP) in the zone of its slip direction and on the shear stress perpendicular to the slip direction. The former relates to the twinning-antitwining asymmetry that has been observed in virtually all bcc metals \( \{1 \overline{1} \} \). The latter represents a non-glide stress that modifies the structure of the dislocation core and thus increases or decreases the Peierls stress.

We have shown previously using a series of uniaxial loadings \( \{6\} \) that no other stress components affect the dislocation glide. This conclusion disagrees with the recent proposal of Koester et al. \( \{7\} \) that the Peierls stress of bcc iron depends explicitly on three normal components, two of which are perpendicular and one parallel to the dislocation line. The objective of this paper is to resolve this controversy by carrying out a series of molecular statics simulations of an isolated 1/2⟨111⟩ screw dislocation under stress and to identify uniquely the stress components that affect its glide. Although all these calculations have been made using the Bond Order Potential (BOP) \( \{8, 9\} \) parameterized for bcc tungsten by Mrovec et al. \( \{10\} \), the conclusions drawn from these studies should be valid generally for all bcc metals. This is supported by recent calculations made by Chen et al. \( \{11, 12\} \) using a magnetic BOP for bcc iron \( \{13\} \) whose results are very similar to those obtained by us previously for bcc molybdenum and tungsten \( \{6\} \).

2. Atomistic simulations

All atomistic simulations carried out in this paper utilized a tetragonal simulation block whose orientation, and thus the coordinate system in which the loading was applied, were defined by the Cartesian axes \( x = [121] \), \( y = [101] \), and \( z = [111] \). Periodic boundary conditions were imposed along the \( z \) direction to simulate a straight infinite 1/2⟨111⟩ screw dislocation, while the widths of the block in the \( x \) and \( y \) directions were about \( 30a \), where \( a = 3.1652 \) Å is the lattice parameter of bcc tungsten. The dislocation was inserted into the middle of the block by shifting all atoms according to the anisotropic linear-elastic strain field of the dislocation that was derived originally by Eshelby, Read and Shockley \( \{14\} \) (for details and further references, see Chapters 13-3 or 13-7 in Hirth and Lothe \( \{15\} \)). The atoms in the region \( 10 < |x|/a \leq 15 \) and \( 10 < |y|/a \leq 15 \), called hereafter the inactive part, were...
then held fixed while the atoms in the region for which \(|x|/a \leq 10\) and \(|y|/a \leq 10\) (active part) were relaxed by molecular statics using the BOP for bcc tungsten [10].

The most general stress tensor that can be applied to the block contains six independent components. Two of these are the shear stresses parallel to the slip direction – one (\(\sigma_{13}\)) acts in the (121) plane, while the other (\(\sigma_{23}\)) in the (101) plane. The remaining four stress components are the shear stress perpendicular to the slip direction (\(\sigma_{12}\)) and the three normal stress components in the direction of the coordinate axes or, equivalently, the hydrostatic stress \(\sigma_h\), the normal stress parallel to the dislocation line (\(\sigma_{33}\)) and one of the remaining two stress components (\(\sigma_{11}\) or \(\sigma_{22}\)).

In the following, we will consider that the MRSSP coincides with the (101) plane. This means that the stress component \(\sigma_{13}\) is zero and the value of \(\sigma_{23}\) at which the dislocation starts to move is the critical resolved shear stress (CRSS). Our objective is to investigate the dependence of the CRSS on the hydrostatic stress \(\sigma_h\), the normal stress \(\sigma_{33}\) parallel to the dislocation line, and the collective effect of the remaining two stress components, \(\sigma_{11}\) and \(\sigma_{22}\). For completeness, we also study the effect of \(\sigma_{12}\) and explain how it affects the CRSS when the MRSSP deviates away from the (101) plane.

### 2.1. Dependence of the CRSS on individual stresses

We begin by investigating the dependence of the CRSS on the hydrostatic stress. Starting with the relaxed atomic block with the dislocation, we further displace all atoms by the stress tensor \(\Sigma_h = \text{diag}(\sigma_h, \sigma_h, \sigma_h)\), where the arguments of \(\text{diag}\) are the three components along the principal diagonal of \(\Sigma_h\). We obtained relaxed atomic blocks for the values \(\sigma_h = \{0, \pm 0.01, \pm 0.02, \pm 0.03\}C_{44}\) in which the atoms in the outer (inactive) region of the block remain displaced by the superposition of the displacement fields of the dislocation and the stress tensor \(\Sigma_h\). In order to investigate the dependence of the CRSS on the hydrostatic stress, we have subsequently superimposed on each of these relaxed blocks the stress tensor

\[
\Sigma_{23} = \begin{bmatrix}
0 & 0 & 0 \\
0 & 0 & \sigma_{23} \\
0 & \sigma_{23} & 0
\end{bmatrix}.
\]

The stress \(\sigma_{23}\) was increased from zero in steps of 0.001\(C_{44}\), while keeping the stress \(\sigma_h\) fixed. The value of \(\sigma_{23}\) at which the dislocation starts to move is then identified with the CRSS. The obtained CRSS vs. \(\sigma_h\) data, plotted in Fig. 1 by blue circles, show that the CRSS is independent of the hydrostatic stress.

We now perform an analogous calculation to investigate the dependence of the CRSS on the stress component \(\sigma_{33}\), i.e. the normal stress that acts parallel to the dislocation line. Starting with the relaxed atomic block with the dislocation, we apply the stress tensor \(\Sigma_{33} = \text{diag}(0, 0, \sigma_{33})\) for the same six values of \(\sigma_{33}\) used when studying the role of the hydrostatic stress \(\sigma_h\). The dependence of the CRSS on the stress component \(\sigma_{33}\) is then obtained by superimposing on a fixed stress tensor \(\Sigma_{33}\) the stress tensor \([1]\) in steps until \(\sigma_{23}\) reaches the CRSS. The obtained CRSS vs. \(\sigma_{33}\) data, plotted in Fig. 1 by blue dots, shows that the CRSS does not depend on the stress component \(\sigma_{33}\).

Based on their recent molecular statics calculations on bcc iron, Koester et al. [7] argued that the CRSS depends on all three normal components along the principal diagonal of the stress tensor. It was shown in Refs. [5, 11, 12] that the 1/2(111) screw dislocations in different bcc metals respond similarly to the applied load and thus the conclusions made in Ref. [7] should be applicable also to bcc tungsten. However, this is not the case because we do not observe any dependence of the CRSS on \(\sigma_h\) and \(\sigma_{33}\). This implies that the only diagonal stress tensor that may affect the CRSS is \(\Sigma_r = \text{diag}(−\tau, \tau, 0)\). This stress tensor imposes a shear stress perpendicular to the slip direction, which can be seen more clearly after rotating the coordinate system by −45° in the zone of the z axis (i.e. in the direction from the (101) plane towards the (011) plane).

The dependence of the CRSS on \(\tau\), published already in Ref. [4], is plotted in Fig. 1 by black filled squares.

To further demonstrate that the CRSS does not depend independently on the two remaining normal stresses \(\sigma_{11}\) and \(\sigma_{22}\), let us consider two stress tensors \(\Sigma_{11} = \text{diag}(\sigma_{11}, 0, 0)\) and \(\Sigma_{22} = \text{diag}(0, \sigma_{22}, 0)\) that impose these loadings. We have shown above that the independence of the CRSS on the hydrostatic stress \(\sigma_h\) and on the stress component \(\sigma_{33}\) means that the CRSS can depend only on a stress tensor that applies an equibiaxial tension-compression in the xy plane. Hence, the relevant part of the stress tensor \(\Sigma_{11}\) is the deviatoric stress \(\Sigma_{11} = \text{diag}(\sigma_{11}/2, −\sigma_{11}/2, 0)\). Similarly, only the deviatoric part \(\Sigma_{22} = \text{diag}(−\sigma_{22}/2, \sigma_{22}/2, 0)\) of the stress tensor \(\Sigma_{22}\) can affect the dislocation glide. Comparisons of these stress

![Figure 1: Dependence of the CRSS on individual components of the stress tensor. The black symbols represent the CRSS vs. \(\tau\) dependence published previously in Ref. [4]; this is further refined here to allow for a point-wise comparison of the CRSS for an equibiaxial tension-compression in the xy plane with the CRSS vs. \(\sigma_{11}\) and the CRSS vs. \(\sigma_{22}\) dependencies.](image-url)
tensors with $\Sigma_r$ above lead to the following observations: (i) loading by the normal stress $\sigma_{11}$ is equivalent to imposing the shear stress perpendicular to the slip direction $\tau = -\sigma_{11}/2$, and (ii) loading by the normal stress $\sigma_{22}$ is equivalent to applying $\tau = \sigma_{22}/2$.

In order to substantiate these conclusions, we have calculated the variation of the CRSS with the stress components $\sigma_{11}$ and $\sigma_{22}$ and compared them to the dependencies of the CRSS on $\tau$ obtained earlier \cite{6}. These calculations were done similarly as above, when investigating the effects of $\sigma_h$ and $\sigma_{33}$. The obtained dependencies of CRSS on $\sigma_{11}$ and $\sigma_{22}$ are plotted in Fig. 1 by the red and green empty triangles, respectively. The CRSS values obtained by applying the stress tensors $\Sigma_{11}$ and $\Sigma_{22}$, plotted in Fig. 1 by the red and green filled triangles, respectively, are derived from the CRSS vs. $\tau$ data that are plotted in this figure by the black squares. One can clearly see that the dependencies in red and green plotted in Fig. 1 by like colors are essentially identical\footnote{The small differences in the CRSS values are comparable with the error bars of the incremental estimate of the CRSS by atomistic simulations.} which validates our observations above.

![Figure 2](image.png)

Figure 2: Changes of differential displacement maps upon applying the stresses (a) $\sigma_{11} = 0.03C_{44}$, and (b) $\sigma_{22} = 0.03C_{44}$. The plane of the figure coincides with the (111) plane and the lattice site that contains the center of the dislocation is marked by the triangle. The red “+” (blue “−”) symbols represent the increase (decrease) of the screw components of the differential displacement map upon incorporating the stress into the relaxed block with the dislocation. If $\sigma_{22} < 0$, the core changes are the same as those in (a), while for $\sigma_{11} < 0$ they are indistinguishable from the figure (b).

For completeness, the plots in Fig. 2 show the regions in which the screw component of the differential displacement map \footnote{The small differences in the CRSS values are comparable with the error bars of the incremental estimate of the CRSS by atomistic simulations.} is increased (red “+” symbols) and decreased (blue “−” symbols) upon applying positive stresses $\sigma_{11}$ and $\sigma_{22}$ using the stress tensors $\Sigma_{11}$ and $\Sigma_{22}$, respectively. The size of each symbol represents the magnitude of an increase or a decrease of this screw component. It follows from Fig. 2, that the effect of $\sigma_{11} > 0$ is to extend the dislocation core on the (011) and (110) planes and constrict it on the (101) plane. We have demonstrated already in Ref. \cite{6} that the same distortion of the dislocation core is caused by a negative applied shear stress $\tau$. Similarly, Fig. 2 shows that the effect of $\sigma_{22} > 0$ is to extend the dislocation core on the (101) plane and constrict it on the other two {110} planes of the [111] zone. Again, this agrees with the effect of positive $\tau$ on the dislocation core, as discussed in Ref. \cite{6}. The comparisons above provide ample evidence that the normal stresses $\sigma_{11}$ and $\sigma_{22}$ should not be thought of as acting in isolation. Instead, they act concomitantly by imposing an equibiaxial tension-compression in the $xy$ plane and manifest themselves by the dependence of the CRSS on the stress $\tau$ that induces shear in the plane perpendicular to the slip direction.

2.2. Dependence of the CRSS on stress combinations

In the following, we will investigate a combined effect of $\tau$ and $\sigma_{33}$ on the CRSS. The initial simulation blocks for these calculations have been obtained by first applying the stress $\tau$ in steps, as before. By keeping this stress constant, we then imposed the stress $\sigma_{33}$ in the same steps until the block was subjected to the desired combination \{ $\tau$, $\sigma_{33}$ \}. Starting with this stressed block, the shear stress parallel to the slip direction ($\sigma_{23}$) was applied as before until the dislocation moved; this value of $\sigma_{23}$ then represents the CRSS for a given combination of $\tau$ and $\sigma_{33}$. These calculations have been made for the values of $\tau/C_{44} = \{0, \pm 0.01, \pm 0.02, \pm 0.03\}$ and $\sigma_{33}/C_{44} = \{0, \pm 0.03\}$. It is important to emphasize that each stress state that imposes a nonzero value of $\sigma_{33}$ applies at the same time a hydrostatic stress $\sigma_h = \sigma_{33}/3$.

![Figure 3](image.png)

Figure 3: Dependence of the CRSS on the shear stress perpendicular to the slip direction ($\tau$) for three values of the stress component $\sigma_{33}$ (and the corresponding hydrostatic stress $\sigma_h$). The black symbols represent a dislocation glide on the (011) plane, while the blue symbols a glide on the (011) plane.

The obtained dependencies of the CRSS on $\tau$ for the three values of $\sigma_{33}$ (and the corresponding $\sigma_h$) are plotted in Fig. 3. This figure clearly shows that the presence of the stress $\sigma_{33}$ has no effect on the CRSS vs. $\tau$ dependence. This observation further proves our assertion that the stress components $\sigma_{33}$ and $\sigma_h$ do not play any role in the glide of 1/2(111) screw dislocations in bcc tungsten. This conclusion should be valid generally for all bcc metals and most likely also for other materials in which the
plastic deformation is governed by the dislocations that possess non-planar cores.

3. Orientational effects of the CRSS and $\tau$

In the calculations above, we considered that the MRSSP coincides with the (101) plane, which is the [110] plane of the [111] zone with the highest Schmid stress. Similar calculations can be carried out for any orientation of the MRSSP, i.e. for any angle $\chi$ that the MRSSP makes with the (101) plane. The loading is then defined in the right-handed orthogonal coordinate system in which the $y'$ axis is perpendicular to the MRSSP and the $z'$ axis parallel to the [111] direction. Any applied load can be expressed in this system as a combination of the stress $\tau$ and the shear stress $\sigma$ parallel to the slip direction and the shear stress $\sigma$ parallel to the slip direction, where

$$\Sigma_{MRSSP} = \begin{bmatrix} -\tau & 0 & 0 \\ 0 & \tau & \sigma \\ 0 & \sigma & 0 \end{bmatrix}.$$  \hspace{1cm} (2)

In atomistic simulations, the stress tensor above has to be resolved in the orientation of the atomic block, where the $y$ axis is perpendicular to the (101) plane and $z \equiv z'$. This transformation constitutes a simple rotation of the coordinate system by $-\chi$ around the [111] axis. The transformed stress tensor

$$\Sigma^{(101)} = \begin{bmatrix} -\tau \cos 2 \chi & \tau \sin 2 \chi & \sigma \sin \chi \\ \tau \sin 2 \chi & \tau \cos 2 \chi & \sigma \cos \chi \\ \sigma \sin \chi & \sigma \cos \chi & 0 \end{bmatrix}$$ \hspace{1cm} (3)

is then used to impose the applied load by displacing all atoms in the simulated cell. In the following, the superscript will refer to the coordinate system in which the stress component is resolved. For example, $\Sigma^{(hkl)}$ refers to a right-handed orthogonal coordinate system with the $z'$ axis parallel to the [111] direction, and the $y'$ axis parallel to the [hkl] direction.

One can immediately see that for $\chi \neq 0$, the shear stress $\sigma$ parallel to the slip direction and applied in the MRSSP acts in the orientation of the simulated block by the glide stress $\sigma_{23}^{(101)} = \sigma \cos \chi$ and by the non-glide stress $\sigma_{13}^{(101)} = \sigma \sin \chi$. If the dislocation glide was not affected by the stress component $\sigma_{13}^{(101)}$, the CRSS would be proportional to $1/\cos \chi$ and would thus be symmetric about $\chi = 0$. This is not the case in bcc metals and the observed twinning-antitwining asymmetry of the CRSS is attributed to the effect of the stress component $\sigma_{13}^{(101)}$. This implies that two terms are needed in the yield criterion to describe the orientational dependence of the shear stress parallel to the slip direction.

Similarly, for $\chi \neq 0$, the stress $\tau$ acts by a pair of normal stresses $\sigma_{22}^{(101)} = -\sigma_{11}^{(101)} = \tau \cos 2 \chi$ and by the shear stress $\sigma_{12}^{(101)} = \tau \sin 2 \chi$. The effect of the latter is to modify the CRSS vs. $\tau$ dependence as the angle of the MRSSP deviates from $\chi = 0$ and, possibly, to alter the slip plane on which the dislocation moves. To demonstrate the effect of the shear stress $\sigma_{12}^{(101)}$, we will consider in the following the MRSSPs (945) and (549) that make angles $\chi \approx \pm 26^\circ$ with the (101) plane. Instead of calculating the CRSS vs. $\tau$ dependence using the full stress tensor (3), we will now artificially set the component $\sigma_{12}^{(101)}$ to zero. The obtained data are plotted in Fig. 3 by empty symbols and interpolated by thin lines. For comparison, our previous results [6] obtained using the full stress tensor (3) are plotted in this figure by filled symbols (thick lines). The observed differences of the CRSS at both positive and negative $\tau$ reveal that the stress component $\sigma_{12}^{(101)}$ cannot be neglected. Its presence promotes the composite (or zig-zag) slip of the dislocation on two (110) planes around $\tau/C_{14} = -0.01$, which gives rise to an average slip plane of the (112) type. These observations suggest that the CRSS and the orientation of the actual slip plane depend both on the magnitude of $\tau$ and on the orientation of the MRSSP.

![Figure 4: The CRSS vs. $\tau$ dependencies calculated for the MRSSPs with angles $\chi \approx -26^\circ$ (upper panel) and $\chi \approx +26^\circ$ (lower panel). The filled symbols (thick lines) correspond to the data obtained using the full stress tensor (3), while the empty symbols (thin lines) are obtained using (3) in which $\sigma_{12}^{(101)}$ is artificially set to zero. The colors distinguish different slip planes in the [111] zone; the two (112) slips are composed of alternating steps of the dislocation on two adjacent (110) planes.](image)

The analysis above implies that the yield criterion for bcc metals has to contain four stress components. Two of these are the shear stresses parallel to the slip direction resolved in two arbitrary (but non-coplanar) planes of the [111] zone. In the yield criterion that we have developed in Ref. [10], the shear stress parallel to the slip direction was resolved in the (101) and (011) planes as $\sigma_{23}^{(101)} = \text{CRSS} \cos \chi$ and $\sigma_{23}^{(011)} = \text{CRSS} \cos (\chi + \pi/3)$. The effect of the shear stress perpendicular to the slip direction, investigated in the atomistic simulations by applying the equibiaxial tension-compression, i.e. $\tau$ in Eq. (2), is in-
corporated in the yield criterion by two shear stresses $\sigma_{12}$ acting in the same two $\{110\}$ planes as above. In particular, $\sigma_{12}^{(10)} = \sin 2\chi$ and $\sigma_{12}^{(20)} = \cos(2\chi + \pi/6)$. Nevertheless, it should be emphasized that these planes need not be the same as those considered above when describing the orientational dependence of the shear stress parallel to the slip direction. The simplest yield criterion for bcc metals can thus be written as a linear combination of the four stress components, identified above, i.e.

$$
\sigma_{23}^{(10)} + a_1\sigma_{23}^{(01)} + a_2\sigma_{12}^{(10)} + a_3\sigma_{12}^{(20)} = \tau_{cr}^*.
$$

(4)

The coefficients $a_1$, $a_2$, $a_3$ and the critical stress $\tau_{cr}^*$ are obtained in Ref. [10] by fitting the atomistically calculated data of CRSS vs. $\chi$ and CRSS vs. $\tau$ for a number of orientations of the MRSSP.

4. Conclusions

The objective of this paper has been to identify the stress components that affect the CRSS to move an isolated $1/2[111]$ screw dislocation in bcc metals in molecular statics calculations. We have shown that the CRSS does not depend on the hydrostatic stress and the stress component $\sigma_{33}$ that is parallel to the dislocation line. The latter observation contradicts the conclusions made in Ref. [2]. It thus follows that the Peierls stress cannot depend directly on the two remaining normal stresses $\sigma_{11}$ and $\sigma_{22}$ but only on their combination represented by the stress tensor $\Sigma = \text{diag}(-\tau, \tau, 0)$, which applies the shear stress perpendicular to the slip direction. The importance of this stress component has been recognized already by Ito and Vitek [4] and quantified fully for bcc molybdenum and tungsten in Ref. [10]. Here, we were able to reproduce the trend in the dependence of the CRSS on the stress components $\sigma_{11}$ and $\sigma_{22}$, calculated for bcc iron by Koester et al. [7]. However, owing to the observation above, we conclude that these dependencies are the manifestations of the dependence of the CRSS on the shear stress perpendicular to the slip direction.

The conclusions of the work of Koester et al. [7] have been recently adopted by Lim et al. [17] to develop a yield criterion and a crystal plasticity finite element model for various bcc metals both of which explicitly contain the effects of normal stresses $\sigma_{11}$, $\sigma_{22}$, and $\sigma_{33}$. They argue that the yield criterion that we have developed in Ref. [10] to describe the onset of yielding in bcc molybdenum and tungsten and which follows from the non-associated flow theory developed in Refs. [18, 19] has to be augmented by other terms that incorporate the effects of the three normal stresses, while keeping the hydrostatic stress zero. However, the calculations made in this paper provide a convincing proof that there is no influence of $\sigma_{33}$ on the CRSS, while both remaining normal stresses act via the shear stress perpendicular to the slip direction.

We have shown in this paper that only four stress components affect the glide of $1/2[111]$ screw dislocations in bcc metals for any orientation of the MRSSP. Two of these are the shear stresses $\sigma_{23}$ parallel to the slip direction resolved in two different planes of the $\{111\}$ zone. Their role is to represent the twinning-antitwining asymmetry of the CRSS. The other two are the shear stresses $\sigma_{12}$ perpendicular to the slip direction, again acting in two different planes of the $\{111\}$ zone but not necessarily the same as the two shear stresses parallel to the slip direction above. The shear stresses perpendicular to the slip direction affect not only the CRSS but also the slip plane on which the dislocation moves at larger negative values of $\tau$. The onset of yielding in bcc single crystals can thus be described by yield criteria that involve linear combinations of these four stress components, as demonstrated for bcc molybdenum and tungsten in Ref. [10]. The calculations made in this paper prove that these yield criteria are complete and, contrary to the assertions of Koester et al. [7] and Lim et al. [17], there are no effects of other stress components besides those considered in the formulation developed in Ref. [10].

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\[ \Delta r(\chi, \tau) \]

- \( \chi = +26° \)
- \( \chi = -26° \)
- \( \chi = 0 \)

- (110) slip
- (211) slip
- (011) slip
- (112) slip