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Core structure of screw dislocations in body-centred cubic metals: relation to symmetry and interatomic bonding

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ABSTRACT

In this paper we discuss both the crystallographic aspects that govern the general features of the cores of $\frac{1}{2}\langle 111\rangle$ screw dislocations in bcc metals and the role of interatomic bonding that is specific to given materials. This analysis is carried out by comparing the results of two atomistic calculations of dislocations in molybdenum, one performed using many-body central force potentials and the other bond-order potentials that include the angular dependence of interatomic interactions. In both cases the core spreads into three $\{110\}$ planes of the [111] zone but in one case it is unique and invariant with respect to the $\langle 101\rangle$ type diad, a symmetry operation of the bcc lattice, and in the second case two distinct configurations exist that are related by the diad operation. Which of the structures is found depends on interatomic interactions and it is shown that the γ surface for $\{110\}$ planes can be used to predict the type of the core spreading. We then demonstrate that both core structures may lead to very similar responses of the dislocation to applied stresses since the strained crystal loses the original symmetry, in particular the corresponding $\langle 101\rangle$ type diad, and thus the distinction between the two types of core vanishes. Finally, we discuss the generality of these concepts when analysing dislocation cores in materials with other structures than bcc.

§ 1. INTRODUCTION

In the earlier developments of the dislocation theory, core effects were considered to be of secondary importance. However, this attitude has changed radically as the research in crystal plasticity moved from close-packed metals to materials with more complex and open structures. It is now generally recognized that core phenomena often lead to unexpected deformation modes, strong and unusual dependence of the flow stress on temperature and strain rate, and to surprising dependences on the orientation of the crystal with respect to the loading axes. The bcc metals and alloys were the first materials in which such effects were recognized and Basinski's group at the National Research Council of Canada in Ottawa stood in the forefront of such studies and carried out some of the first atomic-level modelling of dislocations that control the plastic behaviour of these materials.

The most significant aspects of the plastic behaviour of bcc metals are the above-mentioned features that can be associated with properties of dislocation

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cores (for reviews see Christian (1970, 1983), Kubin (1982), Taylor (1992) and Seeger (1995)). It was the dependence of the yield stress on the orientation of the crystal relative to the loading axes and associated breakdown of the Schmid law that was the 'unusual' behaviour noted already almost 80 years ago by G. I. Taylor who studied yielding in α-iron and β-brass, both of which crystallize in the bcc type structures (Taylor and Elam 1926, Taylor 1928). In the late 1950s, Basinski and Christian (1960) made the very important observation that the strain rate and temperature sensitivity of the flow and yield stress in bcc iron does not vary systematically with the strain. This implies that the density of obstacles that are being overcome with the aid of thermal activation does not increase monotonically with straining, which is in contrast with observations in fcc metals where it increases incessantly with increasing strain (Blewitt *et al.* 1955, Niewczas *et al.* 2001). This is one of the first observations that formed a basis for the notion that some intrinsic obstacles, such as the lattice friction stress (Peierls stress), are responsible for temperature and strain-rate dependence of the flow stress of bcc metals.

As first suggested by Hirsch (1960) and firmly established by many experimental and theoretical studies performed in the last 40 years, such an intrinsic obstacle is the core of $\frac{1}{2}\langle 111\rangle$ screw dislocations that may spread into several planes of the $\langle 111\rangle$ zone. It is then responsible not only for the high lattice friction stress but also for all the outstanding features of the slip geometry and orientation dependences of the yield stress (for reviews see Christian (1983), Duesbery (1989), Duesbery and Vitek (1998), Takeuchi (1999) and Duesbery *et al.* (2002)). This basic characteristic of screw dislocations relates to the crystallography of the bcc lattice and is, therefore, common to all bcc crystals, regardless of the details of the interatomic bonding. The most prominent aspects of the deformation behaviour of bcc materials that relate to properties of screw dislocations are the characteristic temperature and strain-rate dependence of the flow stress and the twinning–antitwinning asymmetry of the yield and flow stresses (for example Duesbery (1989) and Christian (1983)). These have, indeed, been found in a variety of transition metals (for example Mitchell *et al.* (1963), Mitchell and Spitzig (1965), Bowen *et al.* (1967), Foxall *et al.* (1967), Duesbery and Foxall (1969), Statham *et al.* (1970), Irwin *et al.* (1974), Nagakawa and Meshii (1981) and Seeger and Hollang (2000)), alkali metals (for example Kirchner (1978), Basinski *et al.* (1981), Saka and Taylor (1982), Siedersleben and Taylor (1989) and Pichl and Krystian (1997a,b)) and even in the molecular crystal hexamine that crystallizes in the bcc structure (Dipersio and Escaig 1977). However, the quantitative aspects of these properties as well as other unusual behaviour such as yield asymmetries not related to the sense of shearing vary significantly from material to material. Thus, the structure and properties of the core of $\frac{1}{2}\langle 111\rangle$ screw dislocations are in any given material an interplay between crystallographic and bonding aspects. Distinction of these two aspects and recognition of their relative significance are important for fundamental understanding of the plastic properties of different bcc metals.

Atomistic studies of $\frac{1}{2}[111]$ screw dislocation in bcc metals that were carried out using pair potentials (Vitek *et al.* 1970, Basinski *et al.* 1971, 1981, Duesbery *et al.* 1973, Vitek 1974, Seeger and Wüthrich 1976, Duesbery and Basinski 1993), many-body central force potentials (Duesbery and Vitek 1998, Ito and Vitek 2001, Duesbery *et al.* 2002), tight-binding and other approaches that include explicitly the electronic structure (Masuda and Sato 1978, Xu and Moriarty 1996, Rao and Woodward 2001, Yang *et al.* 2001a,b, Mrovec 2002) and most recently by *ab-initio*

density functional theory (DFT)-based methods (IsmailBeigi and Arias 2000, Woodward and Rao 2001, 2002, Frederiksen and Jacobsen 2003), all revealed nonplanar cores and the twinning–antitwinning asymmetry of the critical stress at which the dislocation starts to move. However, two distinct core configurations were found in different studies of nominally the same materials. In both cases the core spreads into three {110} planes of the [111] zone but, in one case, it is unique and invariant with respect to the $[10\bar{1}]$ diad, a symmetry operation of the bcc lattice and, in the second case, two distinct configurations exist that are related by the diad operation (Duesbery 1989, Duesbery and Vitek 1998)†. Obviously, which of these two structures is found depends on the details of atomic interactions.

In this paper we first discuss the crystallographic aspects that govern the general features of the cores of $\frac{1}{2}\langle 111\rangle$ screw dislocations in bcc crystals. This is followed by the analysis of the interplay between crystallography and interatomic bonding specific for given materials. It is shown that the latter can be analysed using the concept of the γ surface (Vitek 1968, 1992, Duesbery 1989) for {110} planes into which the core spreads. We then demonstrate that both core structures may lead to very similar responses of the dislocation to applied stresses since the strained crystal loses the original symmetry, in particular the $[10\bar{1}]$ diad, and thus the distinction between the two types of core vanishes. Finally, we discuss the generality of these concepts when analysing dislocation cores in materials with other structures than bcc. The method of atomistic modelling of dislocation cores, both in the unstressed crystal and under the externally applied stresses, was the same as in previous studies (for example Duesbery and Vitek (1998) and Ito and Vitek (2001)) and its description is not repeated in this paper.

§ 2. Crystallography and energetics of dislocation cores

The most important crystallographic feature affecting the core structure of $\frac{1}{2}[111]$ screw dislocations in bcc crystals is that [111] is the direction of a threefold screw axis in this structure. This was first emphasized by Suzuki (1968) who argued that these dislocations must possess such symmetry and are thus intrinsically nonplanar, for example in the form proposed earlier by Hirsch (1960). Indeed, following the so-called Neumann's (1885) principle, the symmetry of any physical property of a crystal must include the symmetry elements of the point group of this crystal. Since properties are commonly controlled by crystal defects (e.g. plastic flow is governed by dislocations), the same symmetry argument must apply to their structures. Nonetheless, this does not imply that the structure of every crystal defect must be invariant to all point symmetry operations associated with a given structure. If the structure of a defect is not invariant with respect to a point symmetry operation, alternative (energetically equivalent) configurations exist that are related by this symmetry operation. In the case of the $\frac{1}{2}[111]$ screw dislocation, three equivalent configurations would always exist if this dislocation dissociated into partial dislocations either on one {110} or one {112} plane. Indeed, in the early stages of studies of dislocations in bcc metals, such splittings were proposed on both {110} and {112} planes (Cohen *et al*. 1962, Sleeswyk 1963, Kroupa and Vitek 1967). As seen in figure 1, three {110} and three {112} planes belong to the [111] zone and planar splittings of

†In the [111] projection, which is used when depicting the core, the former structure appears as sixfold and the latter as threefold.

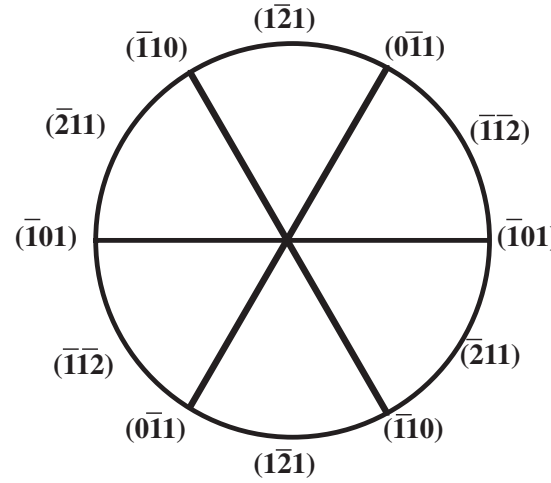

Figure 1. [111] stereographic projection showing orientations of all {110} and {112} planes belonging to the [111] zone.

the $\frac{1}{2}$[111] screw dislocation in either {110} or {112} planes would represent three energetically degenerate configurations.

However, no splitting of dislocations in bcc metals has ever been observed and it is generally accepted that, in these materials, dissociation of dislocations into well-defined partials does not exist. The reason is that there are no metastable stacking faults that could participate in such dissociations. Theoretically, the search for possible stacking faults has been carried out using the concept of the γ surface. This theoretical construct represents the energy of a 'generalized' stacking fault, formed by displacing the two parts of the crystal relative to each other along a crystal plane, as a function of this displacement (Vitek 1968, 1974, 1992, Duesbery 1989). Minima on such a surface determine possible metastable stacking faults. It should be noted that in fcc crystals the γ surface for {111} planes always possesses an extremum for the displacement corresponding to the intrinsic stacking fault for symmetry reasons; three {110} mirror planes intersect at this position. This extremum is a minimum because for this displacement the first and second neighbours remain in the same distances as in the ideal fcc lattice. Thus, the existence of a metastable intrinsic stacking fault is symmetry dictated in fcc crystals. No such symmetry-dictated minimum is present on γ surfaces for either {110} or {112} planes in bcc crystals. This does not mean that metastable stacking faults cannot exist on these planes in principle but, if they did, they would not be common to all bcc crystals but would occur only in some, depending on the details of interatomic bonding. Many calculations of γ surfaces in various bcc metals have been made employing descriptions of interatomic forces ranging from pair potentials to *ab-initio* DFT-based methods (Vitek 1968, 1974, Basinski *et al.* 1971, Duesbery 1989, Medvedeva *et al.* 1996, Duesbery and Vitek 1998, Xu and Moriarty 1998, Mryasov and Freeman 1999, Yang *et al.* 2001a,b, Frederiksen and Jacobsen 2003) and none of these suggests any possible metastable stacking fault.

Since splitting of the $\frac{1}{2}$[111] screw dislocation into well-defined partials and stacking faults is excluded, the core structure is most likely to retain the symmetry consistent with the threefold screw axis of the [111] direction. Atomistic calculations

that employed a wide variety of descriptions of interatomic interactions all confirmed this symmetry of the core. Nevertheless, two types of core were discovered. The first, shown in figure 2, was found in the early pair-potential studies (Vitek *et al.* 1970, Basinski *et al.* 1971, 1981, Duesbery *et al.* 1973, Vitek 1974) as well as in more recent calculations employing many-body central force potentials for molybdenum and tungsten (Duesbery and Vitek 1998, Ito and Vitek 2001, Duesbery *et al.* 2002) and multi-ion interatomic potentials for molybdenum and tantalum derived from first-principles generalized pseudopotential theory (Xu and Moriarty 1996, 1998, Yang *et al.* 2001a,b). The second type of core, shown in figure 3, was also found in some studies using pair potentials (Minami *et al.* 1972, 1974, Kuramoto *et al.* 1974), tight-binding calculations (Masuda and Sato 1978, Sato and Masuda 1981),

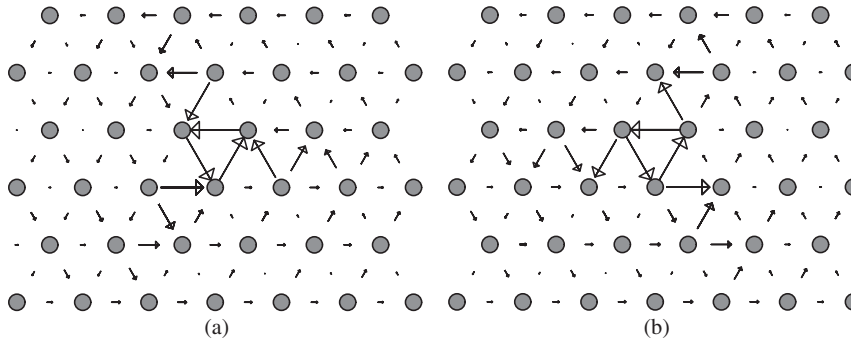

Figure 2. Core structure of the $\frac{1}{2}[111]$ screw dislocation found when using the Finnis–Sinclair-type central-force many-body potentials for molybdenum. The structures presented in (*a*) and (*b*) respectively are related by the symmetry operation of the $[10\bar{1}]$ diad. In this and the following figures we employ the usual differential displacement maps to depict the core structures. The atomic arrangement is shown in the projection perpendicular to the direction of the dislocation line ([111]) and circles represent atoms within one period, without distinguishing their positions in three successive (111) planes. The [111] (screw) component of the relative displacement of the neighbouring atoms produced by the dislocation is depicted as an arrow between them. The length of the arrows is proportional to the magnitude of these components. The arrows, which indicate out-of-plane displacements, are always drawn along the line connecting neighbouring atoms and their length is normalized such that it is equal to the separation of these atoms in the projection when the magnitude of their relative displacement is equal to $\left|\frac{1}{6}[111]\right|$.

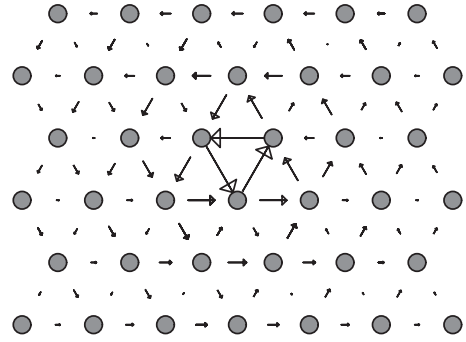

Figure 3. Core structure of the $\frac{1}{2}[111]$ screw dislocation found when using the BOP for molybdenum.

many-body central force potentials for tantalum and niobium (Duesbery and Vitek 1998, Ito and Vitek 2001), *ab-initio* DFT-based calculations for molybdenum and tantalum (IsmailBeigi and Arias 2000, Woodward and Rao 2001, 2002) and other transition metals (Frederiksen and Jacobsen 2003), as well as in calculations employing the recently constructed bond-order potential (BOP) for molybdenum (Mrovec 2002, Pettifor *et al.* 2002, Mrovec *et al.* 2004). Some of the results obtained using the BOP are presented in this paper. The two cores differ in invariance with respect to another symmetry operation of the bcc lattice, the $[10\bar{1}]$ diad. The core shown in figure 2 is spread asymmetrically into the $(\bar{1}01)$, $(0\bar{1}1)$ and $(\bar{1}10)$ planes that belong to the [111] zone and is not invariant with respect to the $[10\bar{1}]$ diad. Hence, another energetically equivalent configuration related by this symmetry operation exists; these two alternatives are shown in figures 2 (*a*) and (*b*), respectively. Since this core exists in two symmetry-related variants it is called degenerate. Alternatively, it has also been called polarized (Seeger and Wüthrich 1976, Seeger 1995, Yang *et al.* 2001a). This is in contrast with the non-degenerate non-polarized core structure shown in figure 3, which is invariant with respect to the $[10\bar{1}]$ diad. Hence, the principal difference between these two types of core of the $\frac{1}{2}[111]$ screw dislocation is symmetry. Whereas both core structures are invariant with respect to the [111] threefold screw axis, the degenerate core is not invariant with respect to the $[10\bar{1}]$ diad while the non-degenerate core is. Two questions arise in this context. Firstly, what determines whether the former or the latter core structure is preferred? Secondly, will dislocations with these alternative core structures respond differently to applied stresses and will the yielding behaviour in materials with different dislocation cores then be considerably different? The second question will be discussed in the following paragraph.

Obviously, the answer to the first question cannot be sought in crystallography but in the energy differences of the two possible core structures. Duesbery and Vitek (1998) proposed that the preference for one or the other type of core can be assessed using the γ surface for the $\{110\}$ planes into which the core spreads. The core shown in figure 2 can be perceived as a generalized splitting into three fractional dislocations with screw components $\frac{1}{6}[111]$ (Duesbery *et al.* 1973, Duesbery and Vitek 1998), while the core shown in figure 3 can be regarded as a generalized splitting into six fractional dislocations with screw components $\frac{1}{12}[111]$. Fractional dislocations, unlike partial dislocations, do not terminate metastable faults but delimit stacking-fault-like regions consisting of faults that are unstable if considered as extended over a large (infinite) area. Thus the degenerate core of figure 2 consists of three faults corresponding to the displacement $\mathbf{b}/3$ (where $\mathbf{b}$ is the Burgers vector $\frac{1}{2}[111]$), on $(\bar{1}01)$, $(1\bar{1}0)$ and $(01\bar{1})$ planes, and the non-degenerate core of figure 3 consists of six faults corresponding to the displacement $\mathbf{b}/6$ on the same planes. Within this paradigm the energy difference between the two cores can be assessed by comparing the values of the γ surface for these two displacements. Specifically, the degenerate core will be favoured if $3\gamma(\mathbf{b}/3) < 6\gamma(\mathbf{b}/6)$ and vice versa for the non-degenerate core.

As an example, we present here two sets of results for molybdenum. The first was obtained with interatomic interactions represented by central-force many body potentials of the Finnis–Sinclair (1984) type (Ackland and Thetford 1987) and the second using the recently constructed BOPs (Mrovec 2002, Pettifor *et al.* 2002). The core structures of the $\frac{1}{2}[111]$ screw dislocation calculated using these two types of potential are shown in figures 2 and 3, respectively. Figure 4 shows the

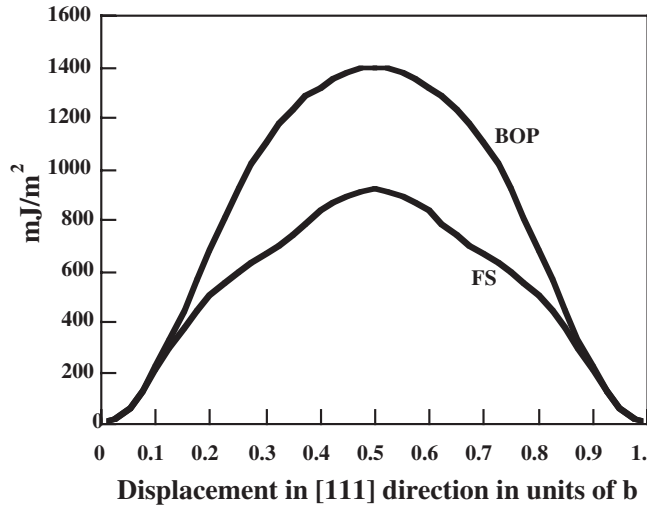

Figure 4. [111] cross-sections of the γ surface for the $(\bar{1}01)$ plane calculated using the Finnis–Sinclair-type central-force many-body potentials for molybdenum (FS) and the BOP respectively.

[111] cross-sections of the corresponding γ surfaces for the $(\bar{1}01)$ plane. From these data, $3\gamma(\mathbf{b}/3)$ equals $2133\,\mathrm{mJ\,m^{-2}}$ for the Finnis–Sinclair type potentials and $3579\,\mathrm{mJ\,m^{-2}}$ for the BOP; The $6\gamma(\mathbf{b}/6)$ values equal $2508\,\mathrm{mJ\,m^{-2}}$ and $3090\,\mathrm{mJ\,m^{-2}}$, respectively. Following the above-mentioned criterion, the degenerate core is favoured for the Finnis–Sinclair-type potentials and the non-degenerate core for the BOP. This is in agreement with the calculated core structures presented in figures 2 and 3. Similarly, the above criterion was found to apply in the case of Finnis–Sinclair-type potentials for molybdenum, tungsten, niobium and tantalum (Duesbery and Vitek 1998) and for six transition metals and iron studied by *ab-initio* DFT-based method (Frederiksen and Jacobsen 2003).

An obvious question arising in this context is why the two descriptions of interatomic interactions in molybdenum lead to such differences in the dislocation core structure and which of these is more appropriate. This can again be answered by analysing the γ surfaces for {110} planes. As seen in figure 4, for displacements smaller than $0.15b$, cross-sections of both γ surfaces are virtually identical. The reason is that this is the harmonic regime and both potentials were fitted to the elastic moduli of molybdenum. However, for larger displacements the γ surface evaluated using the BOP attains appreciably higher values. For these displacements, both the separations of atoms on each side of the corresponding generalized stacking fault and the bond angles are very different from those in the ideal bcc lattice. When calculating the γ surface, relaxation perpendicular to the plane of the fault but not parallel to this plane is carried out since the latter would eliminate the generalized stacking fault. The relaxation perpendicular to the plane of the fault may significantly alter the separations of atoms. In particular, it will eliminate any configuration in which the atoms would be at a distance significantly smaller than the spacing of the nearest neighbours so that their repulsion would be very strong. However, this relaxation will alter only marginally the bond angles. The dependence of the energy on these angles, which originates from the unfilled d band, is included in the BOP scheme, while only the separation of atoms enters the Finnis–Sinclair scheme. Hence,

most probably, it is the angular dependence of the interatomic interactions in the BOP scheme that is responsible for high values of the γ surface at large displacements. As already alluded to, the same non-generate dislocation core as that found using the BOP was also detected in the recent *ab-initio* modelling of screw dislocations in molybdenum (Woodward and Rao 2001, 2002); similarly the γ surface for the $(\bar{1}01)$ plane calculated *ab initio* is very close to that found using the BOP (Freriksen and Jacobsen 2003, C. Woodward, 2003, private communication). Consequently, the non-degenerate core structure, which presumably results from the non-central (angular) character of bonding, appears more appropriate for molybdenum than the degenerate core structure. Since in transitions metals d electrons dominate cohesion (Friedel 1969, Pettifor 1995), the directional character of bonding is generally important and the non-degenerate cores are likely to be more common than the degenerate cores. This has, indeed, been found in the recent *ab-initio* DFT-based calculations of Frederiksen and Jacobsen (2003).

§ 3. Effect of applied stresses and dislocation motion

A detailed atomistic modelling of the effect of applied stresses on $\frac{1}{2}[111]$ screw dislocations was performed by Ito and Vitek (2001) using central-force many-body potentials of the Finnis–Sinclair type for molybdenum and tantalum. As mentioned above, in this case the core is degenerate in molybdenum and non-degenerate in tantalum. A remarkable result of this study is that the responses to the applied stresses are similar for both types of core. Here we focus on the similarities and/or differences in the response of these two types of core to an applied stress by analysing results of atomistic calculations made using the Finnis–Sinclair-type central-force potentials and the BOP for molybdenum; as discussed in the previous section these two descriptions of interatomic interactions yield a degenerate core (figure 2) and a non-degenerate core (figure 3) respectively. The calculations were made for pure shear stress acting in the direction of the Burgers vector with various orientations of the maximum resolved shear stress plane (MRSSP). These orientations are defined by the angle χ which the MRSSP makes with the $(\bar{1}01)$ plane. This representation of the orientation of the MRSSP has been commonly used in earlier theoretical and experimental studies (Christian 1983, Duesbery 1989). Owing to the crystal symmetry it is sufficient to consider $-30^\circ \leqslant \chi \leqslant +30^\circ$; for -30° the MRSSP is the $(\bar{1}\bar{1}2)$ plane, and for $+30^\circ$ the $(\bar{2}11)$ plane. However, it should be noted that orientations corresponding to positive and negative angles χ are not equivalent. In the following, we always give the shear stress acting in the [111] direction as the stress in the MRSSP, and its value when the dislocation starts to move is identified with the critical resolved shear stress (CRSS) for the dislocation glide at 0 K.

In both cases, upon reaching the CRSS, the dislocation started to glide along the $(\bar{1}01)$ plane for all angles χ. The dependence of the CRSS on χ is very similar to that found by Ito and Vitek (2001) (see for example figure 5 of this paper) and, therefore, it is not presented here in detail. The following are some examples of the calculated values of the CRSS. For the Finnis–Sinclair potentials† it is $0.021C_{44}$ for $\chi = 0$, $0.034C_{44}$ for $\chi = +28^\circ$ and $0.020C_{44}$ for $\chi = -28^\circ$; for the BOP it is $0.024C_{44}$ for $\chi = 0$, $0.032C_{44}$ for $\chi = +28^\circ$ and $0.026C_{44}$ for $\chi = -28^\circ$ (for more details see Mrovec

†The values given by Ito and Vitek (2001) are twice as high owing to an unfortunate error that introduced a factor of two into the evaluation of the CRSS.

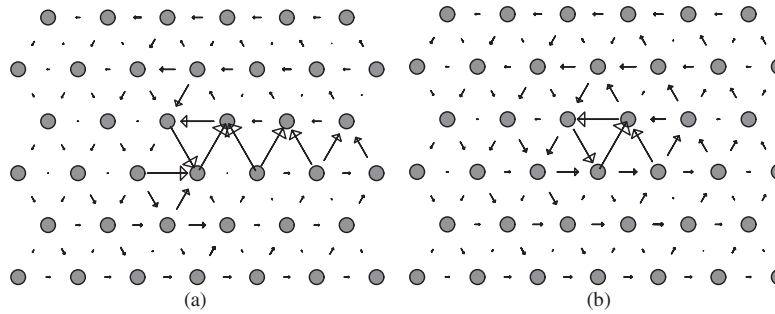

Figure 5. Core structures of the $\frac{1}{2}[111]$ screw dislocation under the effect of the shear stress applied in the MRSSP with $\chi = -28^\circ$. (*a*) Originally the degenerate structure shown in figure 2 (*a*); the applied stress is $0.018C_{44}$. (*b*) Originally the non-degenerate structure shown in figure 3; the applied stress is $0.024C_{44}$.

et al. 2004). Obviously, the values of the CRSS are very similar for both descriptions of atomic interactions and they are also very close to the values obtained by Woodward and Rao (2001, 2002) in *ab-initio* DFT-based calculations.

In general, the CRSS does not obey the Schmid law according to which the dependence of the CRSS on χ should have the form $1/\cos\chi$. It is larger for positive than for negative angles χ, which is related to the twinning–antitwinning asymmetry. For negative χ the nearest {112}-type plane, $(\bar{1}\bar{1}2)$, is sheared in the twinning sense and for positive χ the nearest {112}-type plane, $(\bar{2}11)$, is sheared in the antitwinning sense. However, such asymmetry is not specific to {112} planes but is encountered in all planes of the [111] zone but {110} planes, and it can again be understood on symmetry grounds. In the bcc lattice there is no crystallographic reason why shearing in opposite directions along [111], which is commensurate with changing the sign of the angle χ, should be equivalent. The reason is that {111} planes are not mirror planes in this lattice; {110}-type planes are an exception because the $[10\bar{1}]$ diad assures the symmetry with respect to the sense of shearing for these planes. However, symmetry arguments cannot be used to predict whether the CRSS will be larger for positive than for negative χ or vice versa. The present atomistic calculations, as well as the vast majority of previous studies, predict the former, which is in good agreement with experimental observations (Christian 1970, 1983, Kubin 1982, Duesbery 1989, Taylor 1992).

The reason why the overall behaviours of the $\frac{1}{2}[111]$ screw dislocation under the effect of an applied stress are very similar for the two distinct core structures has to be sought in the changes of the cores induced prior to the dislocation motion by the applied stress. As an example, figures 5 (*a*) and (*b*) show the originally degenerate (figure 2 (*a*)) and non-degenerate (figure 3) cores, respectively, when the shear stress has been applied in the MRSSP with $\chi = -28^\circ$ and the stress levels are somewhat lower than the corresponding CRSS. Both cores now attain a configuration akin to the degenerate structure with displacements spread most extensively into the $(\bar{1}01)$ plane in which the dislocation eventually glides. Most importantly, both these core structures are now unique since the applied stress distorts the lattice such that it removes the symmetry of the $[10\bar{1}]$ diad. Obviously, there is no other structure in the case shown in figure 5 (*b*) since the unstressed non-degenerate structure has already been unique. However, another distorted structure would be obtained in the degenerate case if the starting configuration were that shown in figure 2 (*b*). However, these

two distorted structures would not be symmetry related and thus equivalent. Evidently, the distorted structure which would originate from that of figure 2(*b*) would possess a higher energy and would be more difficult to move (Ito and Vitek 2001). Hence, it is reasonable to assume that it will spontaneously transform into the structure of figure 5(*a*), in particular since, if the two alternate structures exist, it is likely that in the unstressed state the two variants will alternate along the dislocation line, as first suggested by Kroupa (1963).

While the two distorted cores shown in figures 5(*a*) and (*b*), respectively, are unique and similar to each other, they obviously differ in their extensions into {110} planes. This must relate to different types of interatomic interaction employed in the two cases and it can again be rationalized by comparison of the corresponding γ surfaces. The core spreading leads to the formation of generalized unstable stacking faults on {110} planes and, obviously, the extent will be larger, the lower the energy of such faults. As seen from figure 4, such energy is lower in the case of the Finnis–Sinclair potentials than in the case of the BOP, which is congruent with the widths of spreading of the cores shown in figure 5.

§ 4. Discussion

This paper has concentrated on the distinction between crystallographic and energy aspects of the structure and properties of the core of $\frac{1}{2}$[111] screw dislocations in bcc metals, which are the dislocations that control all prominent features of the plastic deformation in these materials. The two symmetry operations most relevant for these dislocations are the threefold screw axis parallel to [111] and the [10$\bar{1}$] diad. The core structure must either be invariant with respect to these two symmetry operations or possess a lower symmetry. In the latter case, energetically degenerate configurations related by the missing symmetry operation exist. Which of these two possibilities arises depends then on interatomic interactions in specific materials.

However, the first most important feature of bcc metals, which is governed by both crystallography and types of interatomic interaction, is that there are no metastable stacking faults that could participate in the conventional splitting of dislocations. The low-index planes on which such stacking faults could be expected are {110} and {112} (Cohen *et al.* 1962, Sleeswyk 1963, Kroupa and Vitek 1967). This was investigated extensively using the concept of γ surfaces (Vitek 1968, 1974, Basinski *et al.* 1971, Duesbery 1989, Medvedeva *et al.* 1996, Duesbery and Vitek 1998, Xu and Moriarty 1998, Mryasov and Freeman 1999, Yang *et al.* 2001a,b, Frederiksen and Jacobsen 2003) but neither calculations employing various model potentials nor calculations fully accounting for the electronic structure of specific metals suggested the existence of such stacking faults. It is important to note that in the bcc structure the existence of such faults is not anticipated on symmetry grounds unlike in fcc materials where the intrinsic stacking fault on {111} planes corresponds to a symmetry-dictated extremum on the γ surface.

Consequently, the $\frac{1}{2}$[111] screw dislocation may not split into well-defined partials but its core may spread into several planes of the [111] zone. The symmetry of such a core is then either lower than or equal to that imposed by the [111] threefold screw axis and the [10$\bar{1}$] diad. Both possibilities, corresponding to the core spreading into {110} planes, were found in atomistic studies and are shown in figures 2 and 3, respectively. Which of these is found in any specific material depends on the details of interatomic bonding and, as described in § 2, the γ surface for {110} planes can be used to make such a prediction. Furthermore, the extent of

the core spreading increases with decreasing height of this γ surface. This analysis may be particularly relevant when studying effects of alloying and, generally, any phenomena that alter the type or strength of bonding. An example is the finding by Yang *et al.* (2001a,b) that the core of the screw dislocation in tantalum is non-degenerate for a negative hydrostatic pressure of 10 GPa, degenerate but only narrowly spread at zero pressure and the spreading of the degenerate core increases significantly with increasing hydrostatic pressure.

However, the ultimate goal of atomistic studies of the cores of screw dislocations in bcc metals is the atomic-level insight into the complex features of the plastic deformation of these materials. From this perspective, the most important is understanding the effect of applied stresses and eventual glide of dislocations. A remarkable result of this study is that the behaviours of the $\frac{1}{2}[111]$ screw dislocations in a strained crystal are very similar for the two alternate core structures. This may be astonishing at first but the analysis of the changes of the core structure induced by applied stresses, combined with symmetry considerations, provides a credible explanation. In the strained crystal, the symmetry associated with the $[10\bar{1}]$ diad is eliminated and both cores attain a unique configuration akin to the degenerate structure. The only difference is the extent of spreading into $\{110\}$ planes that depends on the specific description of interatomic interactions. While in the present paper this effect of the applied stress has been demonstrated only for the shear stress in the direction of the Burgers vector, it is seen from the previous study of Ito and Vitek (2001), where molybdenum displayed a degenerate and tantalum a non-degenerate core, that the same reasoning applies generally, including the application of shear stresses perpendicular to the Burgers vector that cannot move the dislocation but can modify its core.

In this paper the complex stress effects have been identified for infinite straight dislocations and thus, strictly speaking, for dislocations moving as straight lines. This is the case either at very low temperatures or at extreme strain rates. At finite temperatures and usual strain rates the motion of $\frac{1}{2}\langle 111\rangle$ screw dislocations proceeds via formation of pairs of kinks (Duesbery 1989, Seeger 1995). However, the stress dependence of the activation enthalpy of this process can be expected to mimic the stress dependence of the Peierls stress of the straight screw dislocations since in the limit of high stresses, that is very low temperatures or very high strain rates, this mechanism must converge to that of straight dislocations.

Finally, it should be noted that phenomena discussed here are not unique to bcc metals but can be encountered in many different materials, including those with a fcc lattice. In the latter case the Burgers vectors of dislocations are $\frac{1}{2}\langle 110\rangle$ and thus screw dislocations are parallel to fourfold $\langle 110\rangle$ axes. Considering the $[1\bar{1}0]$ direction, there are two $\{111\}$-type planes, (111) and $(11\bar{1})$, belonging to this zone. Since metastable intrinsic stacking faults are always attainable in $\{111\}$ planes, the $\frac{1}{2}[1\bar{1}0]$ screw dislocation will dissociate into Shockley partials on either the (111) or the $(11\bar{1})$ plane, provided that the stacking-fault energy is low enough for this splitting to be energetically favourable. Such dissociations represent a degenerate state of the dislocation. However, if the energy of the intrinsic stacking fault is so high that the splitting is unfavourable, the non-degenerate dislocation core, spread equally into the two $\{111\}$ planes, may be preferred. Such dislocation core is nonplanar and the screw dislocation will then possess attributes akin to those of screw dislocations in bcc metals. This type of dislocation core has not yet been identified in any fcc material. However, it was found in two recent atomistic studies of the ordinary $\frac{1}{2}[1\bar{1}0]$

dislocation in the fcc-based $L1_0$ TiAl alloy, which employed an *ab-initio* DFT-based method (Woodward and Rao 2003) and a bond-order potential for TiAl (Porizek *et al*. 2003, Znam *et al*. 2003) respectively. Another example of dislocations the cores of which may be spread in several non-parallel planes is that of $\frac{1}{2}\langle 331]$ screw dislocations in materials such as $MoSi_2$ with the tetragonal $C11_b$ structure that is formally based on the bcc lattice. The $\{013\}\langle 331]$ system, which is an analogue of the $\{011\}\langle 111\rangle$ system in the bcc lattice, appears to control the plastic deformation of this material at ambient temperatures and thus these dislocations are of principal importance for its ductility (Ito *et al*. 1995, 1996, 1999, Mitchell and Misra 1999). Unlike the situation for $\{110\}$ planes in bcc structures, a number of possible stacking fault-like defects were found by atomistic calculations (Mitchell *et al*. 2001a,b) and considerations based on a hard-spheres model (Paidar and Vitek 2002). Thus $\frac{1}{2}\langle 331]$ screw dislocations may, at least in principle, dissociate on $\{013\}$ planes. However, it is very likely that the energy of the relevant stacking-fault-like defects will be too high for such dissociations to be energetically favoured and in this case these screw dislocations may possess nonplanar cores. The investigation of their structure can then follow the same route as in the case of the cores of screw dislocations in the bcc lattice. In general, nonplanar dislocation cores are likely to be common in non-close-packed structures. The most pertinent approach to exploration of such cores is a crystallographic examination of the symmetries that they have to obey combined with studies of γ surfaces for the planes of possible core spreading. The former applies to any material with a given crystal structure while the latter reflects the main aspects of interatomic bonding in a specific material.

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