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Atomistic simulation of titanium II. Structure of $\frac{1}{3}\langle\bar{1}2\bar{1}0\rangle$ screw dislocations and slip systems in titanium

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ABSTRACT

The bond-order potential for hcp Ti, constructed in part I, and a central-force Finnis–Sinclair-type potential have been used to study atomistically the core structure of the $\frac{1}{3}\langle\bar{1}2\bar{1}0\rangle$ screw dislocation. The qualitative features of the core structures are similar in the two cases. The dislocation may either dissociate into Shockley partials on the basal plane or spread in a continuous manner into the prism plane. However, the spreading of the dislocation core into the prism plane is always energetically favoured over the splitting into the basal plane in the case of the bond-order potential whilst the opposite is found in the case of the central-force Finnis–Sinclair-type potential. Hence, the results obtained using the bond-order potential explain the strong preference for the prism slip over the basal slip in Ti. The most important global parameter is the energy of the intrinsic stacking fault on the basal plane which is so high in the case of the bond-order potential that splitting into Shockley partials is not energetically favourable. The reason for such a high stacking-fault energy is the non-central character of atomic interactions in Ti arising from the significant contribution of d electrons to the bonding, which is correctly captured by the bond-order potential.

§ 1. INTRODUCTION

In all hcp metals the dominant slip direction is the close-packed direction $\langle\bar{1}2\bar{1}0\rangle$ but, unlike in the fcc materials, the close-packed basal plane is not always the favoured slip plane. While it is the principal slip plane in Be, Mg, Zn, Cd and Co, the prism plane is strongly preferred in Ti, Zr, Hf, Y and a number of rare-earth hcp metals (Hirth and Lothe 1982, Legrand 1984b). Considering just the crystal structure, miscellaneous hcp metals differ only in the c/a ratio but this does not correlate with the favoured slip plane. The ideal c/a ratio is 1.633 and both Ti and Zr possess $c/a = 1.59$ which is smaller than but not far from the ideal value. Cd has the largest c/a ratio, 1.89, and Be the smallest, 1.57. Nevertheless, the basal plane is the favoured slip plane in both Cd and Be while the prism plane is favoured in Ti and Zr. However, as first noted by Legrand (1984a, b), the prism plane is generally favoured in transition metals and this preference may depend on the filling of the d band. Indeed, it is the dominant slip plane in Ti, Zr and Hf which all have between 1.5 and 2.5 d electrons, while in Co with more than eight d electrons the basal slip dominates, and in Re and Ru with six to seven d electrons there is no clear preference for the basal or prism slip (Churchman 1954).

For a given slip direction the corresponding dislocations can, in principle, glide on any plane containing this vector. However, in some materials, only one type of slip plane occurs while in others the slip appears on a variety of crystal planes. An example of the former is the fcc class of metals in which {111} slip planes are ubiquitous (Hirth and Lothe 1982), and of the latter the bcc class of metals in which even non-crytallographic slip has been observed (Christian 1983, Duesbery 1989). The reason for this different behaviour is that, in fcc crystals, dislocations always dissociate into Shockley partials on {111} planes while no well defined planar splitting of dislocations exists in bcc metals. On the contrary, $\frac{1}{2}\langle 111\rangle$ screw dislocations possess narrow cores, usually spread into several crystal planes, and can easily cross-slip (Hirsch 1960, Vitek 1975a,1985, Christian 1983, Duesbery 1989). The splitting into partial dislocations and/or spreading of the dislocation core in a single crystallographic plane is generally the reason why such a plane is the dominant slip plane (Vitek 1992). In those hcp metals in which the basal slip dominates, the $\frac{1}{3}\langle \bar{1}2\bar{1}0\rangle$ dislocations indeed split into Shockley partials on the basal plane. Analogously, when the prism slip dominates, we can expect that either splitting or spreading of the dislocation core into the prism plane is favoured. This suggests that, in the transition hcp metals, such as Ti, the covalent bonding induced by the d electrons has a salient control over the core structure of dislocations in that spreading into the prism plane is preferred over splitting into the basal plane.

Consequently, in order to capture the essential features of the core structure of dislocations in Ti (and also Zr, Hf and other hcp transition metals) by atomistic calculations the description of atomic interactions must reflect correctly the covalent character of bonding arising due to the partially filled d band. This is emphasized by the fact that calculations employing pair potentials (Bacon and Martin 1981, Bacon and Liang 1986, Liang and Bacon 1986) or central-force many-body potentials of the embedded-atom method (Oh and Johnson 1988) or Finnis-Sinclair-type potentials (Igarashi *et al.* 1991, Vitek and Igarashi 1991) fail to predict that the prism plane is the dominant slip plane in these metals. The semiempirical method in which the required covalent character of the bonding is included is the parametrized tight-binding method that comprises the two-centre d–d hopping integrals. This approach, combined with the recursion method (Haydock *et al.* 1972, Haydock 1980), was used by Legrand (1984a, b, 1985) in studies of stacking faults and dislocations in Ti. While the results of these calculations do not predict unequivocally the preference for the prism slip, they demonstrate that only if the non-central character of atomic interactions originating from the partially filled d band is included can this preference be attained.

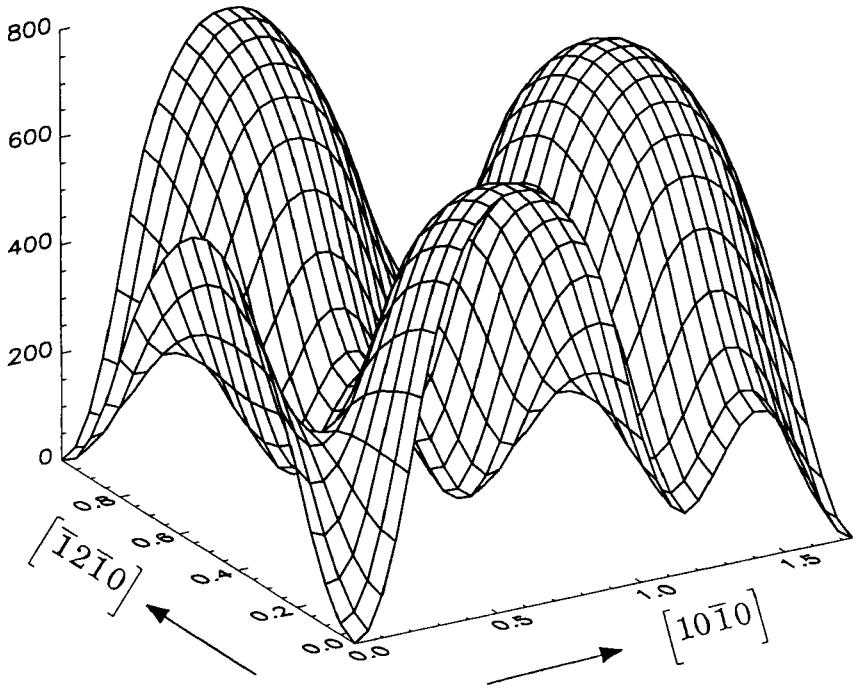
In this paper we investigate the core structure of $\frac{1}{3}\langle \bar{1}2\bar{1}0\rangle$screw dislocations in Ti by atomistic computer simulations. These calculations have been carried out using the bond-order potential presented in part I (Girshick *et al.* 1998), as well as the central-force Finnis–Sinclair-type potential for Ti constructed by Ackland (1992). Results of the two studies are compared in order to expose more prominently the structural and energy aspects governed by the non-central character of the bonding. The most remarkable result is that in the calculations employing the bond-order potential the spreading of the dislocation core into the prism plane is always energetically favoured over the spreading into the basal plane. The opposite is found in the case of the central-force-Finnis–Sinclair-type potential. Hence, the calculations employing bond-order potentials explain the propensity for the prism slip in Ti.

§2. γ SURFACES FOR BASAL AND PRISM PLANES

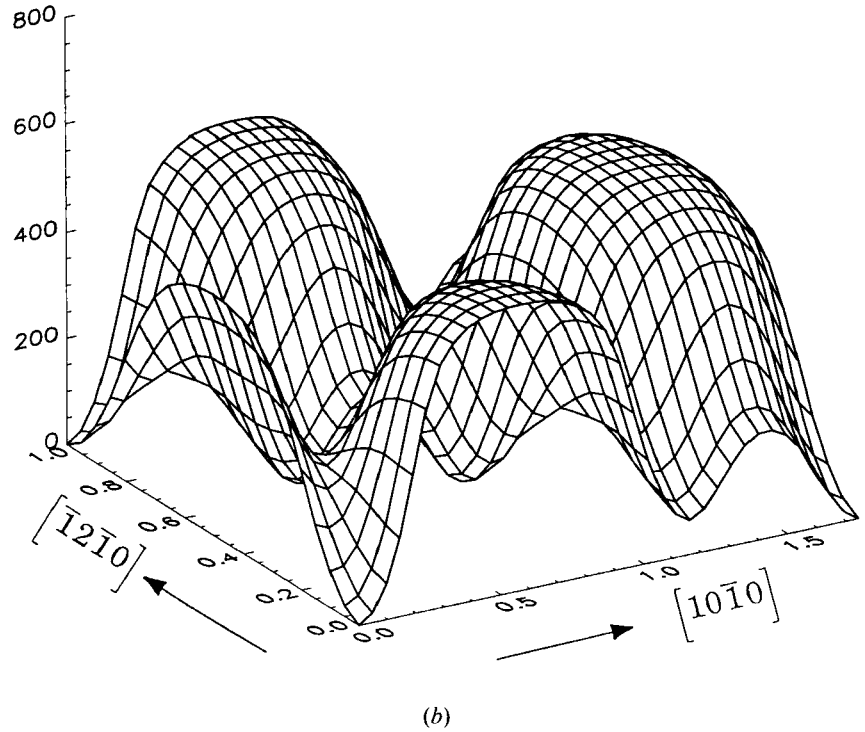
Investigation of γ surfaces, which were first introduced when searching for possible stacking faults in bcc metals (Vitek 1968), is an indispensable precursor for the dislocation core studies (Duesbery and Richardson 1991, Vitek 1992). γ surfaces are energy against displacement surfaces obtained by the following procedure. The crystal is cut along a chosen crystal plane and the upper part displaced with respect to the lower part by a vector **u**, parallel to the plane of the cut. The energy $\gamma(\mathbf{u})$ of a planar fault created in this way is evaluated allowing relaxation perpendicular but not parallel to the fault. The γ surface is then obtained by repeating this procedure for various vectors **u** within the repeat cell of the plane of the cut. The local minima on this surface reveal possible metastable stacking faults on the crystal plane considered and the shape of the γ surface (in particular its first derivatives) determines, the details of the spreading of the cores of dislocations confined to this crystallographic plane (Christian and Vitek 1970, Vitek *et al.* 1972, Vitek 1992, 1996a).

The γ surfaces, calculated using the bond-order potential and the Finnis–Sinclair-type potential for Ti, are shown in figures 1 (*a*) and (*b*) for the basal plane and figures 2 (*a*) and (*b*) for the prism plane. In the case of the basal plane, the γ surfaces found for the two potentials are topologically very similar and the minima on these surfaces correspond to the displacement $\frac{1}{3}[\bar{1}100]$ which defines the well known intrinsic stacking fault. For this displacement the existence of an extremum on the γ surface is guaranteed by symmetry because three mirror planes perpendicular to the basal plane intersect at this position (Yamaguchi *et al.* 1981, Vitek 1992). Since for this displacement the separations of the first and second neighbours are almost unaltered, it can be expected that this extremum is a minimum. Hence, the symmetry of the hexagonal structure guarantees that the intrinsic stacking fault is a metastable fault in all hcp crystals. The energy of this fault is, of course, strongly dependent on interatomic bonding. For the bond order potential the energy of this fault is $110\,\mathrm{mJ\,m^{-2}}$ and for the Finnis–Sinclair-type potential it is $64\,\mathrm{mJ\,m^{-2}}$. This difference in the stacking-fault energies is the first very important distinction between the bond order potential and the central-force Finnis–Sinclair-type potential. Indeed, calculations employing central-force potentials always predict a relatively low energy of the intrinsic stacking fault on the basal plane since the only significant contribution to this energy arises from the third and more distant neighbours. In contrast, when directional bonding is included, interactions within the shell of first neighbours contribute significantly to the energy of this stacking fault.

The second important difference between the γ surfaces determined using the bond-order potential and the central-force Finnis–Sinclair-type potential is that the γ surface for the prism plane does not display any minimum in the former case but a minimum, corresponding to the displacement $\frac{1}{6}[\bar{1}2\bar{1}0] + 0.18[0001]$, is found in the latter case; the energy of this fault is $253\,\mathrm{mJ\,m^{-2}}$. Unlike the intrinsic stacking fault on the basal plane, this possible stacking fault on the prism plane is not a consequence of the symmetry and whether it is metastable or not depends on the details of interatomic bonding. The stabilization of this stacking fault in the case of Finnis–Sinclair-type potential is the consequence of central forces; this fault can be envisaged using the hard-sphere model (Schwartzkopff 1969) and it was, indeed, found in other central-force calculations (Igarashi *et al.* 1991). Both the notably different stacking-fault energies on the basal plane and the qualitatively different γ surfaces for the prism plane found when using the bond-order potential and the central-force

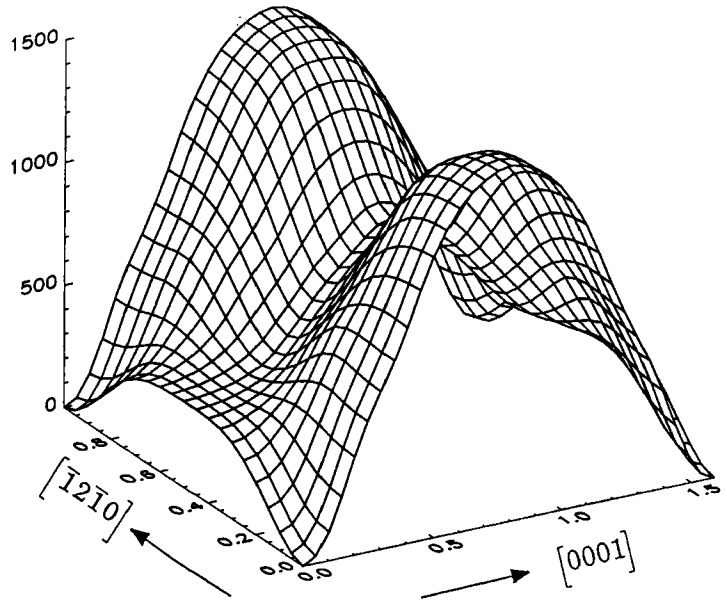


(*a*)

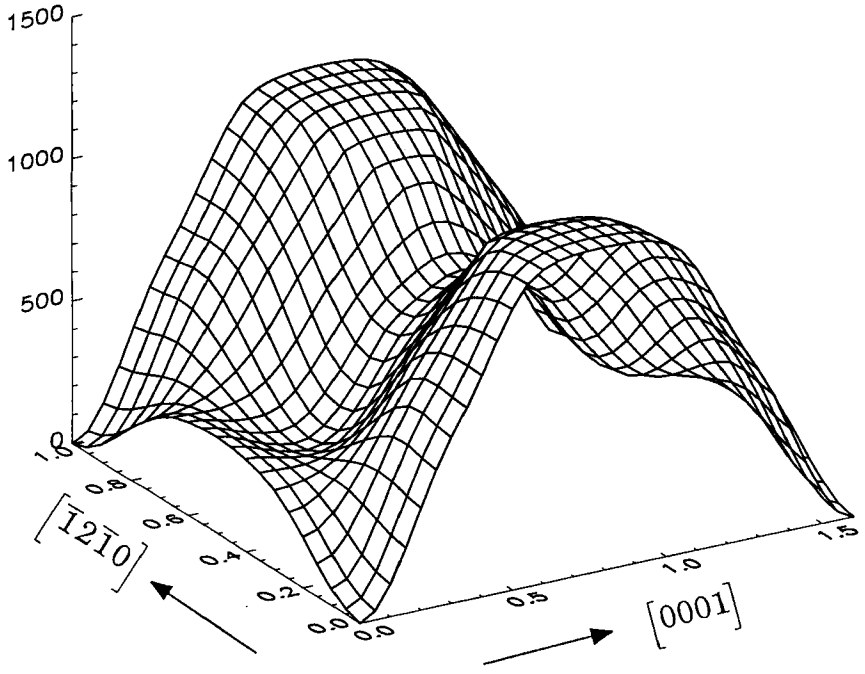


(*b*)

Figure 1. γ surface for the basal plane in Ti calculated using (*a*) the bond-order potential and (*b*) the Finnis–Sinclair-type potential.



(*a*)



(*b*)

Figure 2. γ surface for the prism plane in Ti calculated using (*a*) the bond-order potential and (*b*) Finnis–Sinclair-type potential.

Finnis-Sinclair-type potential suggest that these two schemes may lead to significantly different dislocation core structures. This is investigated in the following studies of dislocation cores.

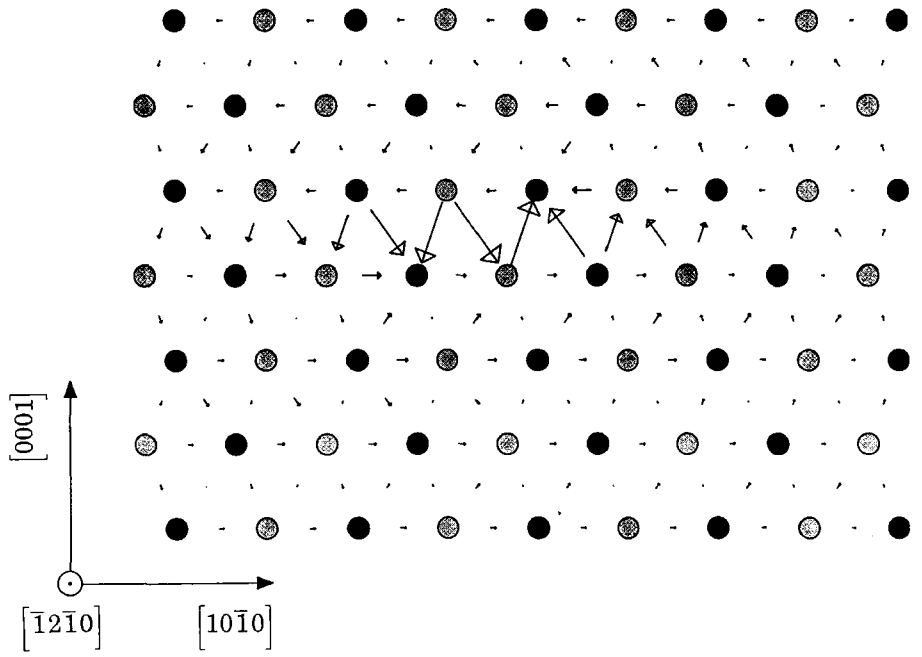
§ 3. The core structure of $\frac{1}{3}[\bar{1}2\bar{1}0]$ screw dislocations

In the hcp structure the most common dislocations carrying the plastic deformation are dislocations with the Burgers vector $\frac{1}{3}[\bar{1}2\bar{1}0]$. They can glide in both basal (0001) and prism $(10\bar{1}0)$ planes. The screw dislocation, lying parallel to the $[\bar{1}2\bar{1}0]$ direction, can spread into either of these planes or into both of them simultaneously. This is the reason why our atomistic studies concentrated on the core structure of this dislocation.

The calculations were carried out using a standard methodology and employing both the bond-order potential and the Finnis–Sinclair-type potentials. A block of atoms was built in the computer and the dislocation introduced into its centre by displacing all the atoms in accordance with the anisotropic elastic displacement field of this dislocation (Hirth and Lothe 1982). The block was then divided into two regions. Atoms in the inner region, which contains the core of the dislocation, were fully relaxed with respect to their positions using a gradient method, while the atoms in the border region were kept at fixed positions. Periodic boundary conditions were employed in the direction parallel to the dislocation line, using the crystal periodicity of the $[\bar{1}2\bar{1}0]$ direction. The relaxed region had dimensions $18a$ in the two directions perpendicular to the dislocation line, where a is the lattice spacing, and it contained 485 atoms. The calculations were always carried out for several starting configurations corresponding to differently positioned centres of the elastic field of the perfect screw dislocation.

In the following the core structures found by this computer modelling are represented using the method of differential displacements that has been commonly employed in dislocation core studies (Vitek *et al.* 1970, Duesbery 1989, Vitek 1992). The atomic arrangement is shown here in the projection onto the plane perpendicular to the direction of the dislocation line, that is the $(\bar{1}2\bar{1}0)$ plane. Open and full circles represent atoms within one period ($\frac{1}{3}[\bar{1}2\bar{1}0]$) along the direction of the dislocation line, positioned at two different levels along this direction. The screw or edge components (parallel and perpendicular to the $[\bar{1}2\bar{1}0]$ direction respectively) of the relative displacement of the neighbouring atoms, produced by the dislocation, are depicted as arrows between them. The length of the arrows is proportional to the magnitude of this displacement and it is normalized such that the length of the largest arrow is equal to the separation of the neighbouring atoms in the $(\bar{1}2\bar{1}0)$ projection. In this scheme, rows of arrows of constant length delineate planar faults, such as stacking faults.

In the case of the bond-order potential simulations, the $\frac{1}{3}[\bar{1}2\bar{1}0]$ screw dislocation always spread into the prism plane, independently of the starting configuration, while in the case of the Finnis–Sinclair-type potential, spreading of the dislocation occurred into either the prism or the basal plane, depending on the position of the elastic centre of the dislocation in the starting configuration. The latter case corresponds to splitting into Shockley partials. For the bond-order potential a metastable configuration corresponding to the same splitting on the basal plane could also be found but only if the partials were introduced via the starting configuration. This structure is shown in figure 3 where both screw and edge components of the displacements are displayed; figure 4 shows the same configuration for the



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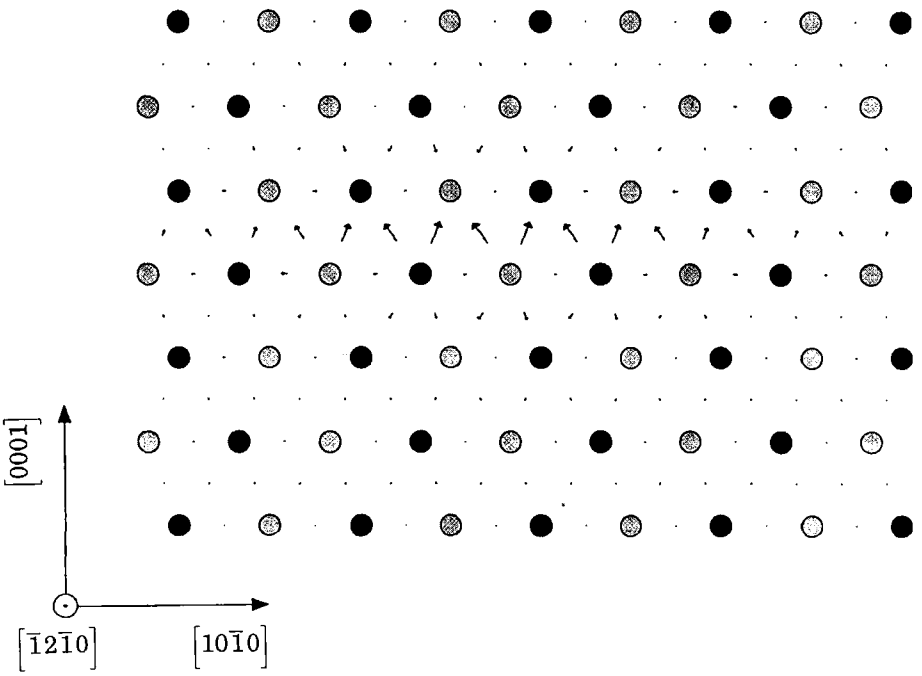
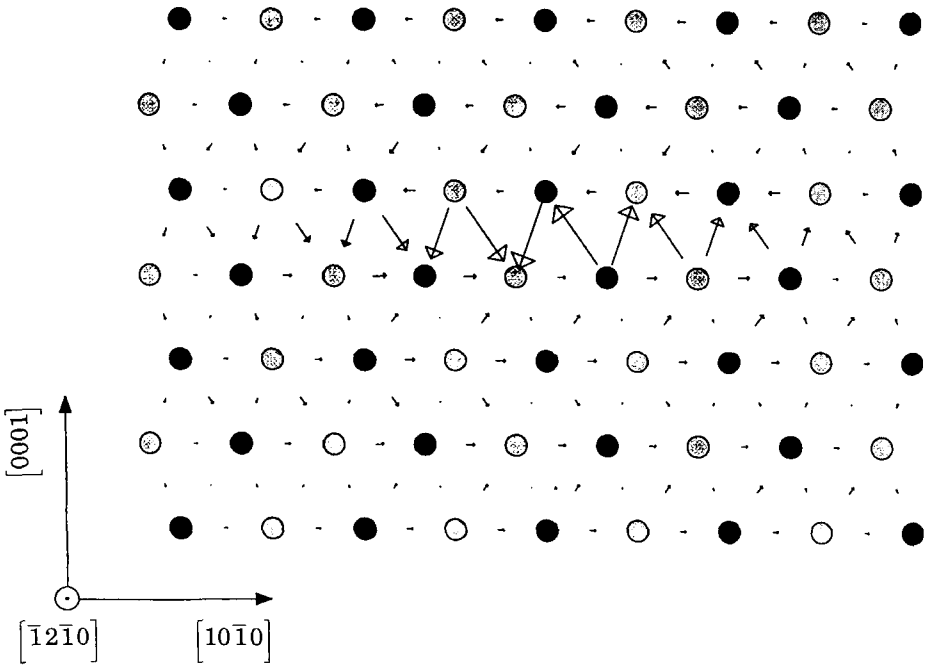
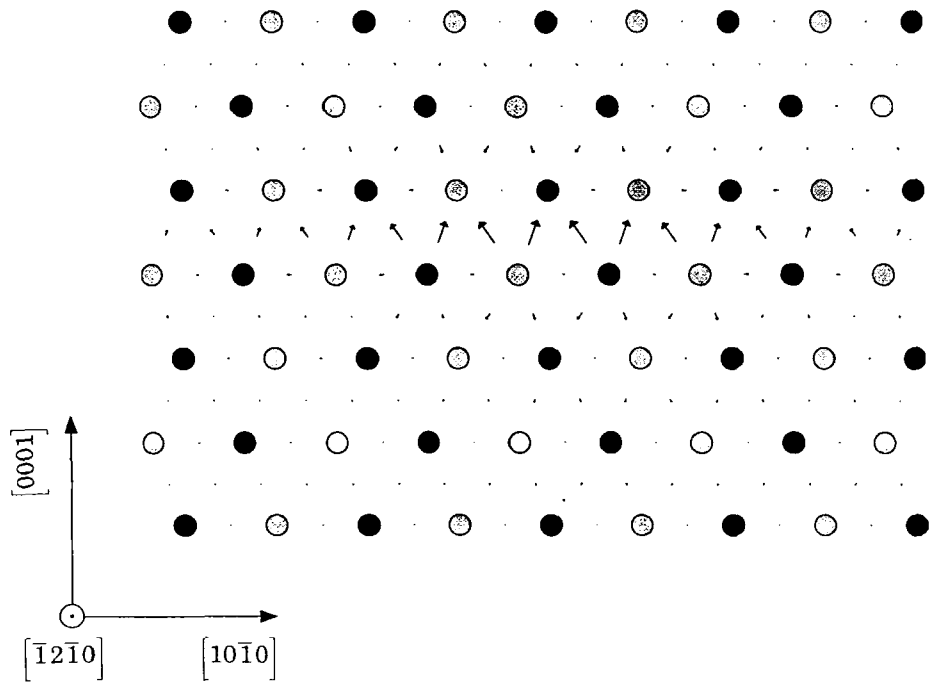


(*b*)

Figure 3. Core of the $\frac{1}{3}[\bar{1}2\bar{1}0]$ screw dislocation spread into the basal plane calculated using the bond-order potential: (*a*) screw component; (*b*) edge component.



(*a*)



(*b*)

Figure 4. Core of the $\frac{1}{3}[\bar{1}2\bar{1}0]$ screw dislocation spread into the basal plane calculated using the Finnis–Sinclair-type potential: (*a*) screw component; (*b*) edge component.

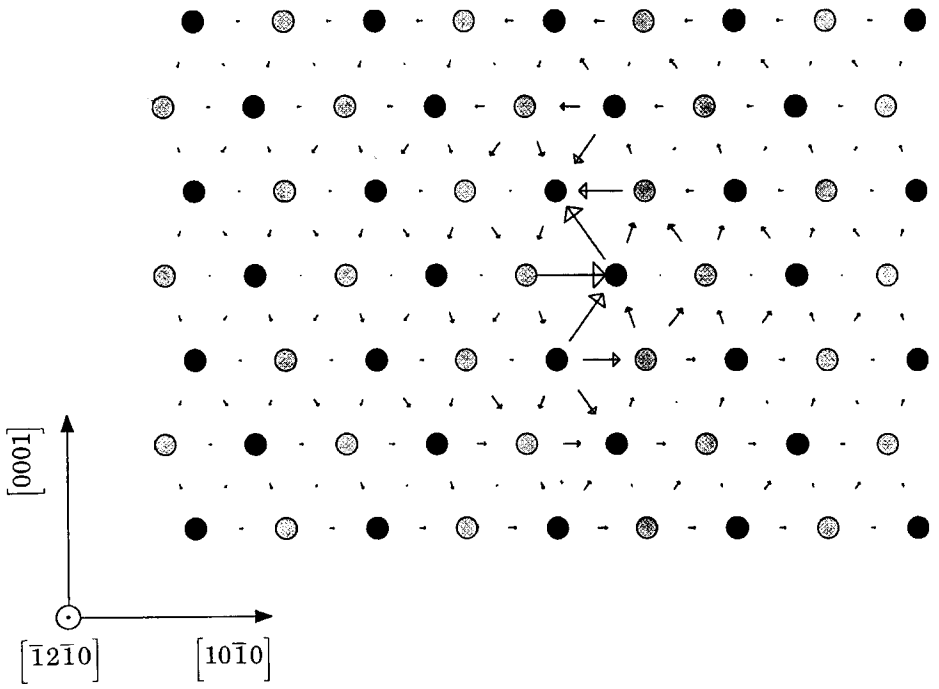


Figure 5. Core of the $\frac{1}{3}[\bar{1}2\bar{1}0]$ screw dislocation spread into the basal plane calculated using the bond-order potential; only the screw component is displayed.

Finnis–Sinclair-type potential. In both cases the edge components are significant, reflecting the fact that the Burgers vectors of the Shockley partials possess components perpendicular to the $[\bar{1}2\bar{1}0]$ direction. This component delineates clearly the region of the stacking fault where it is almost constant.

The core spread into the prism plane was found to be very similar for both the bond-order potential and the Finnis–Sinclair-type potential. Hence, the corresponding structure, shown in figure 5, is displayed only for the case of the bond-order potential simulations; only the screw component is presented since the edge component is negligible. A characteristic feature of this core structure is that, although most of the spreading is into the prism plane, the core is not entirely planar but spreads to some extent into four adjacent (0001) planes. The same feature of the screw dislocation core was also found in calculations of Legrand (1985).

Clearly, the core structures found for the two types of potential are quite similar. In the case of the basal plane, when the core spreading concurs with the splitting into Shockley partials, the core shown in figure 4 is broader than that shown in figure 3. This is obviously related to the fact that for the Finnis–Sinclair-type potential the stacking-fault energy is lower. In the case of spreading into the prism plane, the core configurations found for the two types of potential are essentially identical. These results suggest that the possible forms of the core spreading are generic and do not depend sensitively on the potential used.

The important but more subtle distinction between the two different descriptions of atomic interactions is whether the spreading into the basal or prism plane is preferred energetically. The relaxation calculations suggest that in the case of the bond-order potential the dislocation core spreading into the prism plane is favoured

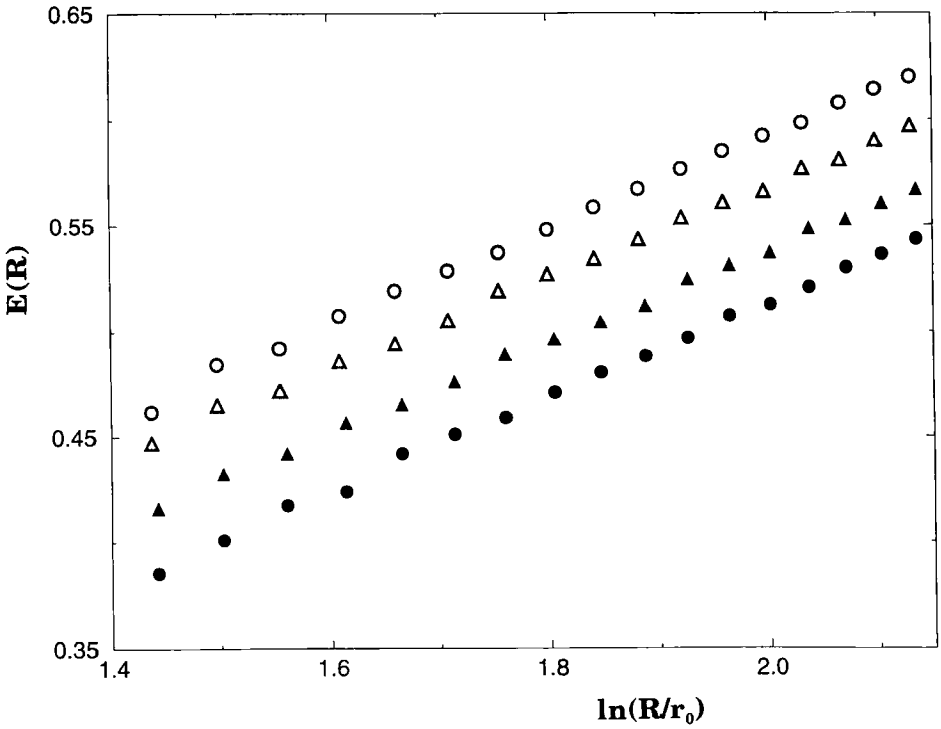


Figure 6. Plot of the energy (in electrovolts per angström) of the $\frac{1}{3}[\bar{1}2\bar{1}0]$ screw dislocation stored within the cylinder of radius R, centred at the dislocation line, against $\ln(R/r_0)$; (●), (▲), the Finnis–Sinclair-type potential; (○), (△), the bond-order potential; (●), (○), core spreading in the basal plane, (▲), (△), core spreading in the prism plane.

since this configuration has been found for all starting configurations. However, this does not imply that the opposite is true for the Finnis–Sinclair-type potential.

In order to analyse the energy preference for core spreading it is necessary to evaluate the dislocation energy in each case. In general, the energy stored within the cylinder of radius R centred on the dislocation line can be written for $R \gg r_0$ as

$$E_{\text{disl}}(R) = \frac{Kb^2}{4\pi} \ln\left(\frac{R}{r_0}\right) + E_{\text{core}}, \tag{1}$$

where E_{core} is the core energy, r_0 the core radius, b the magnitude of the Burgers vector, equal to a in the present case, and K a constant which depends on elastic moduli and the orientation of the dislocation line and the Burgers vector and can be evaluated using the anisotropic theory of elasticity (Hirth and Lothe 1982). Hence, the plot of the energy stored within the cylinder of radius R, centred on the dislocation line, against $\ln R$ will be a straight line for values of R much larger than r_0† and the slope of this line is for a given dislocation independent of the core structure.

† Since the division of the dislocation energy into elastic and core energies is not unique, the choice of the value of r_0 is somewhat arbitrary. In the present calculations, r_0 was set equal to b. E_{core} can then be identified with the value of E_{disl} given by equation (1) for $\ln(R/r_0) = 0$, that is $R = r_0$.

Such plots, evaluated using the corresponding relaxed blocks with the $\frac{1}{3}[\bar{1}2\bar{1}0]$ screw dislocation in the middle, are shown in figure 6. They demonstrate unambiguously that in the case of the bond-order potential the dislocation with the core spread into the prism plane possesses a lower energy than the dislocation with the core spread into the basal plane, whilst the opposite holds in the case of the Finnis–Sinclair-type potential. Hence, although the same core structures are possible in both cases, spreading of the core of the $\frac{1}{3}[\bar{1}2\bar{1}0]$ screw dislocation into the prism plane is favoured in the case of the bond-order potential while in the case of the Finnis–Sinclair type potential the core of the same dislocation prefers to spread into the basal plane in the form of splitting into Shockley partials.

§4. Discussion

The atomistic calculations presented in this paper have been made using the central-force Finnis–Sinclair-type potential and the bond-order potential which reflects the non-central character of bonding in Ti. When considering the core structure, the results are qualitatively very similar for both descriptions of atomic interactions. In both cases the $\frac{1}{3}[\bar{1}2\bar{1}0]$ screw dislocation may either dissociate into Shockley partials on the basal plane or spread in a continuous manner into the prism plane. In the former case the only difference is the width of the splitting which is simply controlled by the energy of the stacking fault on the basal plane. In the latter case the cores are even more similar, possessing almost the same widths and the displacements in the cores are all parallel to the Burgers vector, that is no edge component is present in the core. This is so in spite of the fact that for the Finnis–Sinclair-type potential a metastable stacking fault is available on the prism plane.

However, the quantitative analysis of the two core configurations in terms of the energy of the dislocations clearly differentiates between the two descriptions of atomic interactions. The spreading into the prism plane is favoured in the case of the bond-order potential while for the Finnis–Sinclair-type potential the usual splitting into the basal plane is more favourable. Since the prism slip is strongly preferred in Ti (Hirth and Lothe 1982), the $\frac{1}{3}[\bar{1}2\bar{1}0]$ dislocations carrying the plastic deformation are gliding in prism planes and must be therefore confined to them. Hence, the bond-order potential rather than the central-force Finnis–Sinclair-type potential predicts the dislocation core configuration in agreement with experimental observations. This propounds, as first suggested by Legrand (1984a, b, 1985), that it is the non-central character of bonding controlled by the d electrons that is responsible for the dominance of the prism slip in Ti and, presumably, other hcp transition metals with their partially filled d bands.

Let us consider now the possible dislocation dissociations and core spreadings in more detail. Using the usual continuum theory of dislocations, the width of splitting on the basal plane, determined by the balance of the stacking fault energy and repulsive interaction between Shockley partials, is $5.0a$ for the Finnis–Sinclair-type potential and $2.9a$ for the bond-order potential†; where a is the lattice parameter. As discussed in § 2, a metastable stacking fault is found on the prism plane in the case of the Finnis–Sinclair-type potential. The possible dissociation with this fault would be according to the reaction $\frac{1}{3}[\bar{1}2\bar{1}0] = \frac{1}{6}[\bar{1}2\bar{1}x] + \frac{1}{6}[\bar{1}2\bar{1}\bar{x}]$, where $x \approx 1.08$, and, for the

† In this calculation the anisotropic elasticity and stacking-fault energies corresponding to these potentials, 64 mJ m^{-2} and 110 mJ m^{-2} respectively, were used.

stacking fault energy of $253\,\mathrm{mJ\,m^{-2}}$ the width of splitting is $1.25a$. Such a narrow splitting is not physically meaningful and this is, presumably, the reason why this stacking fault does not play any role in the core structure of dislocations on prism plane.

An alternative to the splitting is a continuous spreading of the core into the prism plane which has been found in the present study again for both types of description of atomic interactions. A similar dislocation core structure has also been found by Legrand (1984b, 1985) who suggested analysing the core spreading in terms of a splitting into two partials with the Burgers vectors $\frac{1}{6}[\bar{1}2\bar{1}0]$ separated by an 'average' stacking fault with the energy $\bar{\gamma}_p = \frac{1}{2}[\gamma(u = 0.2a) + \gamma(u = 0.3a)$. Using the usual elastic analysis it is found that the preference for splitting into the basal or prism plane is in this case controlled by the parameter $\mathcal{R} = C_{66}\gamma_b/C_{44}\bar{\gamma}_p$, where γ_b is the stacking-fault energy on the basal plane. The basal splitting is favoured when $\mathcal{R} < 1$ and the prism splitting when $\mathcal{R} > 1$. From the results of the present study with the bond-order potential $\bar{\gamma}_p = 260\,\mathrm{mJ\,m^{-2}}$ and therefore $\mathcal{R} = 0.4$ (see part I for the elastic moduli). However, the direct evaluation of the energy of the dislocation spread into the prism and basal plane respectively, presented in figure 6, demonstrates that prism spreading is favoured. This means that Legrand's simplified analysis is not adequate for deciding which core structure is favoured energetically.†

Nevertheless, the preference for core spreading is closely related to the stacking-fault energy on the basal plane. The γ surfaces for the prism plane calculated using bond-order potential and the Finnis–Sinclair-type potential respectively are very similar both qualitatively and quantitatively. For example, the magnitude of γ for $u = a/2$ (corresponding to $\frac{1}{6}[\bar{1}2\bar{1}0]$) is $350\,\mathrm{mJ\,m^{-2}}$ for the bond-order potential and $342\,\mathrm{mJ\,m^{-2}}$ for the Finnis–Sinclair-type potential. On the other hand, the stacking fault energy on the basal plane is about 60% lower for the Finnis–Sinclair-type potential. The explanation is that in any central-force scheme with short range interactions the energy of the intrinsic stacking fault on the basal plane is relatively low. The reason is that the separation of the first- and second-nearest neighbours remains almost unchanged when this stacking fault is formed and the first significant change appears at the third-nearest neighbours. One of them increases its separation by about 8%, to a distance approximately equal to that of the fourth-nearest neighbours, and two (formerly fifth) neighbours move closer. On the other hand, on the prism plane, several nearest and second-nearest neighbours change their separations by up to 8%. Thus, only if the change in the energy associated with the interaction of third neighbours is relatively large would a high stacking-fault energy ensue.‡ However, the empirical central-force interaction schemes, including the Finnis–

† A more precise analysis could be made using the Peierls model (for example, Hirth and Lothe (1982)) where the core is described as a continuous distribution of infinitesimal dislocations of density $\rho(x) = \mathrm{d}u/\mathrm{d}x$, where u is the displacement parallel to the Burgers vector and the x coordinate is perpendicular to the dislocation line. This density is then related via the Peierls integral equation to the derivative $\partial\gamma/\partial u$ of the γ surface (Christian and Vitek 1970, Vitek *et al.* 1972, Vitek, 1992, 1996a). However, this analysis is unlikely to provide a deeper insight into the preference for core spreading than the direct evaluation of the dislocation energy presented in figure 6.

‡ A different situation may arise in the case of long-range Friedel oscillations of pair potentials constructed on the basis of weak pseudopotentials (Taylor 1981; Vitek 1996b). For example in Al these oscillations are in phase and lead to a relatively high stacking-fault energy (Vitek 1975b).

Sinclair-type potential employed in this study, are short range, usually not extending beyond fourth neighbours, and the interaction energy decays rapidly with increasing separation of atoms. Hence, the intrinsic stacking-fault energy will be relatively low.

However, in the case of short-range interactions, which is appropriate when the significant part of bonding is due to d electrons, the stacking-fault energy on the basal plane may be high if the bonding is directional since the dihedral angles between first-nearest neighbours change when the fault is formed. This is, presumably, the reason why the energy of the intrinsic stacking fault is in the case of the bond-order potential appreciably higher than in the case of the central forces. Hence, it is the non-central character of atomic interactions in Ti arising because of the significant contribution of d electrons to the bonding, which is correctly captured by the bond-order potential, that is responsible for the preference of prism slip over the basal slip. On the level of more global parameters it is the energy of the intrinsic stacking-fault energy on the basal plane which becomes too high for the usual basal plane splitting to be favoured over core spreading into the prism plane.

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