Stacking faults and the $\gamma$-surface on first-order pyramidal planes in $\alpha$-titanium

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Abstract
Using first principles methods we calculated the entire $\gamma$-surface of the first-order pyramidal planes in $\alpha$-titanium. Slip on these planes involving dislocations with $c + a$-type Burgers vectors is one means by which $\alpha$-titanium polycrystals may supplement slip on prism planes with $a$-type Burgers vectors to maintain ductility. We find one low energy and one high energy stacking fault with energies of 163 mJ/m$^2$ and 681 mJ/m$^2$ respectively. Contrary to previous suggestions [1, 2], we do not find a stable stacking fault at $(c + a)/2$.

KEYWORDS
Titanium; density functional theory; stacking fault; gamma-surface; pyramidal; hexagonal close-packed

PACS CLASSIFICATION
61.72.Nn, 62.20.fk, 62.20.fq, 61.50.Ah

1. Introduction

Titanium and its alloys are used in the aerospace industry owing to their high specific strength, fatigue resistance and corrosion resistance [3]. $\alpha$-titanium has a hexagonal close packed (hcp) crystal structure and it may deform plastically either by slip or twinning. The primary slip planes are $\{1100\}$ prism planes shown in red in Fig. 1 with Burgers vectors $\langle a \rangle = (1/3)(1\bar{1}20)$ in the basal plane [3]. There are only two such independent prism slip systems. At least three additional independent slip systems are required to accommodate an arbitrary deformation, according to the von Mises criterion. More general deformation may be accommodated by twinning, when it is not suppressed by alloying. Alternatively, it may be accommodated by ‘$(c + a)$ slip’ with Burgers vectors $\langle c + a \rangle = \frac{1}{3} (1213)$ on the $\{0\bar{1}1\}$ first-order pyramidal planes, one of which is shown in green in Fig. 1 or on $\{1122\}$ second-order pyramidal planes. There are four independent $\langle c + a \rangle$ slip systems on first-order pyramidal planes; with the two independent prism slip systems the von Mises criterion is satisfied.

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Figure 1.: (Colour online) Some slip planes in α-Ti. The critical resolved shear stress at room temperature is smallest on the prism plane (red) with Burgers vector \( \langle a \rangle \), followed by the basal plane (blue) with Burgers vector \( \langle a \rangle \), and the first-order pyramidal plane (green) for slip with Burgers vector \( \langle c + a \rangle \) [3].

\( \langle c + a \rangle \) dislocations are observed in experiments where single α-Ti crystals are deformed in tension along the \( c \)-axis, and in polycrystals [4,7]. These dislocations have been observed predominantly on \{0111\} planes but they have also been observed on \{1122\} planes. Paton et al. [4] and Minonishi et al. [5] found that \( c \)-axis deformation in α-Ti single crystals below 300°C was predominantly accommodated by twinning with \( \langle c + a \rangle \) slip ahead of the propagating twins. Above 400°C deformation was effected by a combination of twinning and \( \langle c + a \rangle \) slip. Numakura et al. [7] found that all deformation in α-Ti polycrystals along the \( c \)-axis was accommodated by \( \langle c + a \rangle \) slip. They also suggested that \( \langle c + a \rangle \) dislocations may dissociate because the Burgers vector is so large. Tomsett and Bevis observed a dissociation of \( \langle c + a \rangle \) dislocations into a pair of \( (1/2)\langle c + a \rangle \) partial dislocations in Zn [8,9]. We are unaware of any experimental evidence for such a dissociation in α-Ti.

\( \langle c + a \rangle \) dislocations have recently been observed in molecular dynamics (MD) simulations of a Mg single crystal strained along the \( c \)-axis. Tang and El-Awady [10] observed that \( \langle c + a \rangle \) dislocations nucleate via the formation of two partial dislocations: a leading partial with Burgers vector \((1/9)[\bar{3}\bar{2}5]\) and a trailing partial \((1/9)[0\bar{1}1\bar{3}]\).

When a perfect dislocation dissociates into partial dislocations there are stacking faults (SFs) between them. The fault vectors correspond to local minima of an energy surface called the \( \gamma \)-surface [11]. For a given lattice plane normal \( \hat{n} \) one half of the crystal is translated rigidly with respect to the other half by \( t \), where \( t \cdot \hat{n} = 0 \). The \( \gamma \)-surface is the energy \( \gamma(t) \) of the generalised stacking fault with fault vector \( t \). For a rational plane translational symmetry limits the inequivalent set of fault vectors \( t \) to those within the Wigner-Seitz cell of the two-dimensional lattice in the plane. Point group symmetry may reduce the set of inequivalent fault vectors further. Allowing atomic relaxation only along \( \hat{n} \) the energy \( \gamma(t) \) of the fault is calculated at absolute zero. This procedure works particularly well when the spacing of lattice planes with normal \( \hat{n} \) is relatively large. As the lattice plane spacing decreases atomic relaxations parallel to the fault may become increasingly important, in addition to those normal to the fault. It is then essential to carry out a fully unconstrained relaxation of any fault.
that corresponds to a local minimum of $\gamma(t)$ to see whether the minimum still exists and whether its translation vector $t$ changes. A further complication arises in crystals where each lattice site is associated with more than one atom, such as hcp, because there may be more than one distinct separation between atomic planes sharing the same normal. In these circumstances the location of the fault plane is not unique.

The first-order pyramidal plane \{011\} is the plane on which $\langle c + a \rangle$ slip is most often seen in $\alpha$-Ti \cite{7,9,12}. There are two spacings of atomic \{011\} planes in an hcp crystal. In this paper we use first principles methods to compute the entire $\gamma$-surface for a generalised fault lying between \{011\} atomic planes with the larger spacing. Faults between widely spaced \{011\} atomic planes are relevant to $\langle c + a \rangle$ slip, while faults between narrowly spaced \{011\} atomic planes are relevant to $\langle a \rangle$ slip \cite{13}.

Domain and Legris \cite{2} and Kwasi
ciak et al. \cite{1} calculated line sections of the $\gamma$-surface for the \{011\} plane along $a$ and $c + a$ using DFT and a $3p^6d^2s^2$ pseudopotential for $\alpha$-Ti. Their results for generalised faults between widely spaced planes are in good agreement. The $c + a$ line section of the \{1011\}$\gamma$-surface of $\alpha$-Zr calculated by Domain and Legris \cite{2} is very similar to that of $\alpha$-Ti, with a local minimum at $\approx \frac{1}{2} (c + a)$. However, the energy of the minimum was considered \cite{2} probably too high to lead to dissociation of a dislocation with Burgers vector $c + a$ into two with Burgers vectors $\approx \frac{1}{2} (c + a)$. We will show that there is no stable stacking fault in $\alpha$-Ti with a fault vector of $\approx \frac{1}{2} (c + a)$.

Yin et al. \cite{13} used symmetry arguments and a hard sphere model to identify approximate translation vectors of possible stable stacking faults without calculating the full $\gamma$ surfaces. They then carried out full relaxations of these faults using DFT for six hcp metals including Ti. On the first order \{011\} pyramidal plane they considered both widely and narrowly spaced atomic planes. They found two stable stacking faults on the widely spaced planes with energies of 134 mJ/m$^2$ and 634 mJ/m$^2$. In this paper we show that the first of these is the only stable stacking fault between widely spaced \{011\} planes in Ti by calculating the full $\gamma$-surface.

Liang \cite{14} proposed a dissociation of a $c + a$ dislocation based on his stacking fault energy calculations using DFT and the nudged elastic band (NEB) method. He proposed a $\langle c + a \rangle$ dissociation into three partials with Burgers vectors $0.19 \langle 2113 \rangle$, $0.215 \langle 1012 \rangle$ (the twinning direction on the (1011) plane), and $0.072 \langle 1210 \rangle$. The $\langle 1/3 \rangle \langle 1210 \rangle$ vector can lie either in the (1011) plane or the (1010) plane.

The entire $\gamma$-surfaces between both narrowl
ly and widely spaced atomic \{011\} planes have been calculated for $\alpha$-Zr using DFT and an embedded atom potential \cite{15}. They found the maximum energies in the $\gamma$-surface for the narrowly spaced planes were much higher than for the widely spaced planes. Ghazisaeidi et al. \cite{16} calculated the $\gamma$-surface for the narrowly spaced atomic \{011\} planes in $\alpha$-Ti using a modified embedded atom potential, and compared the line section of the surface along $a$ with DFT. Poty et al. \cite{17} also calculated entire $\gamma$-surfaces between closely spaced first order pyramidal planes in $\alpha$-Ti and $\alpha$-Zr using classical interatomic potentials, as well as along the $\langle c + a \rangle$-type direction using DFT. Their results agree qualitatively with the results of Ghazisaeidi et al., but differ quantitatively.

In this paper we present DFT and interatomic potential calculations of the entire $\gamma$-surfaces in $\alpha$-Ti between widely spaced first order pyramidal planes. This study builds upon work carried out using the same interatomic potential which includes the $\gamma$-surfaces on the basal, prism, and first-order pyramidal planes \cite{18}. We have also computed the entire $\gamma$-surface on the basal plane in $\alpha$-Ti, which has already been computed using DFT by Benoit et al. \cite{19} along with the $\gamma$-surface on the prism plane. This comparison of our basal $\gamma$-surface results with those of Benoit et al. provides a
useful check on our calculations. As far as we know the entire DFT $\gamma$-surface between widely-spaced first order pyramidal planes in $\alpha$-Ti has not been previously published.

The computational methods are set out in section 2, the $\gamma$-surfaces are presented in section 3, the discussion of these results follows in section 4, and we conclude in section 5. Additional details concerning the convergence tests carried out in support of the results of this study are detailed in appendices A and B.

2. Methods

2.1. DFT/MD parameters

All DFT results in this paper were obtained using CASTEP version 8.0 [20]. We used two types of ultrasoft pseudopotential for Ti [21]. The first was the pseudopotential with 12 valence electrons in the $3s^23p^63d^24s^2$ ground state configuration (denoted 12elPP) generated by the CASTEP on-the-fly pseudopotential generation tool. The second was the 4 valence electron pseudopotential (4elPP) in the $3d^24s^2$ ground state configuration generated by White [22]. The PBE exchange-correlation functional [23] was used for all calculations.

A plane wave energy cut-off of 480 eV for both the 12elPP and the 4elPP enabled the error in the total energy arising from the incomplete basis set to be reduced to 3 meV/atom. Convergence to 0.5 meV/atom was reached with a 23x23x15 $k$-point mesh for the primitive unit cell using both pseudopotentials. We used the cold smearing scheme [24] to improve computational efficiency with a smearing width of 0.1 eV. We computed energy volume curves for $\alpha$-Ti and fitted them to the Birch-Murnaghan equation of state [25, 26] to determine $a = 2.94$ Å and $c/a = 1.580$. DFT relaxations were deemed complete when the maximum force on any atom was less than 10 meV/Å, and the total electronic energy was converged to within 0.01 meV per atom.

All MD calculations were carried out using LAMMPS [27] and the interatomic potential (IP) generated by Ackland [28]. The IP was used with the equilibrium lattice parameters for which the potential was constructed, i.e. $a = 2.97$ Å and $c/a = 1.592$. IP relaxations were deemed complete when the maximum force on an atom was less than 0.01 meV/Å.

2.2. Supercell geometries: basal

Three dimensional periodic boundary conditions were applied to a supercell comprising 14 atomic basal planes. The smallest rectangular repeat cell in the (0001) plane is bounded by $(1/3)[11\bar{2}0]$ and $[1\bar{1}00]$ lattice vectors (see Figs. 2(a) and 3). This cell contains two lattice sites, one associated with the four corners and one in the centre. A primitive periodic cell in the plane of the generalised fault was selected for the $\gamma$-surface calculation, bounded by $(1/3)[11\bar{2}0]$ and $(1/3)[2\bar{1}\bar{1}0]$. The $\gamma$-surface was sampled using a 78 point uniform grid in this primitive cell. Each supercell contained two equivalent generalised stacking faults with equal and opposite translation vectors. The faults were separated by 7 (0002) planes. See Appendix A for details of convergence tests.

2.3. Supercell geometries: first-order pyramidal

For the $\gamma$-surface on the (1101) first order pyramidal plane a slab geometry was used with the generalised faults in the middle of each slab. Three-dimensional periodic boundary conditions were applied with 26.8 Å vacuum between the slabs. The smallest rectangular repeat cell in the (1101) plane is bounded by $(1/3)[11\bar{2}0]$ and $[1\bar{1}02]$ lattice
Figure 2.: Projected views along [11\overline{2}0] direction of the hcp crystal to illustrate the stacking sequences (a) ... ABAB ... of (0002) basal planes and (b) ... ABCDEFGH ... of (11\overline{1}0) pyramidal planes. Small and large circles distinguish atoms on adjacent (11\overline{2}0) planes. Black and white atoms distinguish atoms on the two hexagonal sublattices in the hcp structure.

vectors. This cell also contains two lattice sites. Exploiting the mirror symmetry normal to [11\overline{2}0] and translational symmetry of the lattice only a quarter of the rectangular cell has to be sampled to construct the full $\gamma$-surface; the cell bounded by $\frac{1}{6}[11\overline{2}0]$ and $\frac{1}{2}[1\overline{1}02]$ was sampled by a uniform $4 \times 12$ uniform grid for both the DFT and IP calculations. However, for the 12elPP $\gamma$-surface a uniform grid of only 24 points was used. The normal to (11\overline{1}0) is not a lattice vector, but a nearby lattice vector is [3\overline{3}0\overline{2}]. In each [3\overline{3}0\overline{2}] repeat there are eight (11\overline{1}0) lattice planes and sixteen (11\overline{1}0) atomic planes (see Fig. 2(b)). The spacings of (11\overline{1}0) atomic planes alternate between small and large. Following Ackland [28], a pair of closely spaced atomic planes is called a ‘superplane’. The slab contained one generalised stacking fault between a pair of adjacent superplanes. Each period of the slab comprised 48 atoms arranged in 12 superplanes.

Before the faults were introduced the slab was relaxed fully. When the generalised stacking faults were introduced the two superplanes furthest from and on either side of the fault were allowed to displace only rigidly normal to the fault, i.e. to float.

See Appendix B for details of the pyramidal convergence tests carried out in support of this study.

3. Results

3.1. The basal $\gamma$-surface

The $\gamma$-surfaces computed for the basal plane using DFT with the 12elPP and an IP[28] are shown in Fig. 3. The local minimum at $\frac{1}{3}[10\overline{1}0]$ on each $\gamma$-surface, and its translational equivalent at $\frac{1}{3}[10\overline{1}0] + \frac{1}{3}[11\overline{2}0] = \frac{1}{3}[21\overline{3}0]$, corresponds to the intrinsic stacking fault. The corresponding intrinsic stacking fault energies (ISFEs) are compared with
Figure 3.: (Colour online) The $\gamma$-surface for the basal plane computed using (a) DFT with the 12elPP and (b) an IP [28]. While the positions of the local maxima and minima are the same in the two $\gamma$-surfaces they have smaller energies in the IP $\gamma$-surface. All energies are expressed in mJ/m$^2$. The contours are spaced by 50 mJ/m$^2$. A primitive unit cell in the basal plane is outlined in black.

Published calculated and experimental values [2, 17, 19] in Table 1. It is striking that the interatomic potentials underestimate the ISFE by up to a factor of five compared with experiment and DFT calculations. This discrepancy has been discussed in previous publications [19, 29]. In recent work it has been shown that this potential fitting procedure can be improved by including basal faults in the set of fitting parameters with the inclusion longer ranged interactions [30].

3.2. The first-order pyramidal $\gamma$-surface

The $\gamma$-surface computed using DFT and the 4elPP is shown in Fig. 4(a). The surface is similar to the $\alpha$-Zr $\gamma$-surface computed by Chaari et al. [15].

The $\gamma$-surface computed using DFT and the 12elPP is very similar to that computed with the 4elPP. Figure 4(c) shows the difference $\gamma_{12\text{elPP}}(t) - \gamma_{4\text{elPP}}(t)$ between the 12elPP and 4elPP $\gamma$-surfaces. This gives a measure of the error associated with using the 4elPP instead of the 12elPP. The dark blue colouring of the entire surface indicates that the error is small throughout. Indeed, the root mean square difference is 27 mJ/m$^2$. However near to the local maxima at [0, 0.4] and [0.5, 0.12], the energy difference reaches 40 mJ/m$^2$. The position of the local minimum in the $\gamma$-surface remained unchanged with the 12elPP.

The vector at the centre of the $\gamma$-surfaces shown in Fig. 4 is $\frac{1}{3}[2\bar{1}13]$, which is a $c+a$ lattice vector. The energy of the $\gamma$-surface at that point is therefore zero. In Fig. 4(a) there is a local minimum at [0.00, 0.22]. This is quite close to what Ackland [28] called an ‘intrinsic’ stacking fault configuration. Hence we call this fault ‘$I_1$’ because the fault can be formed intrinsically either by the above translation or the removal of 2 superplanes. We observe a similar stacking fault at [0, 0.15] in our $\gamma$-surface computed using the IP shown in Fig. 4(b).

Ackland also refers to an ‘extrinsic’ stacking fault which would be located at roughly [0.5, 0.25] on the $\gamma$-surface. The term extrinsic is not appropriate here since the fault may be created by relative translation at a single plane. Hence we shall label this fault ‘$I_2$’ instead, consistent with our labelling of $I_1$. A local minimum consistent with the
Figure 4.: (Colour online) $\gamma$-surfaces of the first-order pyramidal plane computed using (a) DFT with the 4elPP and (b) an IP [28]. The energy scale for both $\gamma$-surfaces is shown on the right. All energies are expressed in mJ/m$^2$, and the contours are separated by 50 mJ/m$^2$. The difference between the DFT $\gamma$-surfaces computed with the 4elPP and 12elPP is plotted in (c), where the contours are separated by 10 mJ/m$^2$, and contours of negative energy are shown by broken lines.
Table 1.: Intrinsic stacking fault energies (ISFE) on the basal plane computed in this work and elsewhere compared with experiment. Results have been separated into DFT, tight binding (TB), bond order potential (BO), interatomic potentials (IP, ZM, HKV, A-FS, MEAM).

<table>
<thead>
<tr>
<th>Results</th>
<th>ISFE (mJ/m²)</th>
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<tbody>
<tr>
<td>DFT (this work)</td>
<td>306</td>
</tr>
<tr>
<td>DFT [19]</td>
<td>259</td>
</tr>
<tr>
<td>DFT [2, 16]</td>
<td>292</td>
</tr>
<tr>
<td>DFT [13]</td>
<td>306</td>
</tr>
<tr>
<td>TB [31, 32]</td>
<td>290-370</td>
</tr>
<tr>
<td>IP (this work)</td>
<td>65</td>
</tr>
<tr>
<td>ZM [19]</td>
<td>54</td>
</tr>
<tr>
<td>ZM [33]</td>
<td>56</td>
</tr>
<tr>
<td>HKV [19]</td>
<td>65</td>
</tr>
<tr>
<td>A-FS [29]</td>
<td>64</td>
</tr>
<tr>
<td>BO [29]</td>
<td>110</td>
</tr>
<tr>
<td>MEAM [34]</td>
<td>170-172</td>
</tr>
</tbody>
</table>

Experiment [35] >300

expected location of \( I_2 \) on the \( \gamma \)-surface is observed at \([0.5, 0.26]\) of Fig. 4(b). However, in Fig. 4(a) the \( \gamma \)-surface displays a saddle point at this location, not a local minimum. This was confirmed by refining the contour spacing to 25 mJ/m². Therefore we do not find this is a stable fault in DFT when relaxation is allowed only normal to the fault plane. We will show below that the fault is metastable near this translation state when relaxations parallel to the fault plane are permitted.

The energies of the faults are given in Table 2 where they are compared to values obtained by other groups. Values of the stacking fault energies are given for (i) relaxation displacements constrained to be normal to the fault plane only and (ii) relaxations normal and parallel to the fault are permitted (shown as ‘Con’ and ‘Full’ respectively in Table 2). For the fully relaxed \( I_1 \) fault using DFT we obtain energies of 150 mJ/m² with the 4elPP and 163 mJ/m² with the 12elPP. With only half the energy of the intrinsic stacking fault on the basal plane the energy of the \( I_1 \) fault is remarkably small. We find a metastable fault corresponding to \( I_2 \) at \([0.5,0.26]\) once full relaxation is permitted. We confirmed its instability by perturbing the translation of the fault along the [11 20] direction, following which it relaxed to the \( I_1 \) fault. We obtain energies of 700 mJ/m² with the 4elPP and 681 mJ/m² with the 12elPP. Our fault energies are all slightly higher than those obtained by Yin et al. [13] and by Liang [14].

Following full relaxation we find the translation vector of the \( I_1 \) fault is \([0.0, 0.22]\) in agreement with Yin et al. [13], while for the \( I_2 \) fault we obtain \([0.5,0.26]\) for the translation vector in the fully relaxed state, differing slightly from \([0.5,0.24]\) reported by Yin et al. [13].

The \( I_1 \) fault energies decrease significantly after unconstrained ‘Full’ relaxation.
The differences are nearly a factor of two. To investigate the source of these large differences in $I_1$ we compared the structures of both faults obtained by DFT using the 12elPP with constrained and full relaxations. The differences were extremely small, with changes in the translation vector parallel to the $I_1$ fault of $[0.00, 0.02]$ Å, and a contraction perpendicular to the fault of $0.10$ Å facilitated by small local relaxations.

When the saddle point configuration becomes the local minimum corresponding to the $I_2$ fault the energy decreases by only 15%. In this case there was an expansion of the slab of $0.10$ Å perpendicular to the fault. The differences along $[1102]$ were as large as $0.19$ Å on either side of the geometrical fault plane, decreasing to $0.07$ Å at the surfaces.

Figure 5(a) shows the fully relaxed slab obtained with the 12elPP. The structure consists of a contiguous array of octahedra and tetrahedra, examples of which are shown by ‘o’ and ‘t’. The free (1101) surfaces at the top and bottom of the slab undergo small inward relaxations, and their structures also comprise contiguous arrays of slightly distorted octahedra and tetrahedra.

Fig. 5(b) shows the atomic structure of the fully relaxed $I_1$ fault obtained with the 12elPP. The atomic structure of the fault comprises a contiguous array of octahedra shown by ‘o’ with tetrahedra (not shown) filling the remaining space. The superplanes adjacent to the fault are less rumpled than in the bulk.

Fig. 5(c) shows the atomic structure of the fully relaxed $I_2$ fault obtained with the 12elPP. Part of the displacement associated with this fault is along the direction of projection, which transforms small circles into large circles and vice versa. As a result the atomic structure of the fault comprises an array of trigonal prisms and tetrahedra, shown by ‘p’ and ‘t’.

In the $\gamma$-surface obtained with the IP the $I_1$ point was found to have an energy of 233 mJ/m$^2$. The energy reduced to 225 mJ/m$^2$ when an unconstrained relaxation was performed. The $I_2$ stacking fault has an energy of 377 mJ/m$^2$, which reduced to 351 mJ/m$^2$ when an unconstrained relaxation was carried out.

The changes in the energies of the faults between the constrained and unconstrained
Results

<table>
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<tr>
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<th>$I_1$</th>
<th>$I_2$</th>
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<tbody>
<tr>
<td></td>
<td>Full</td>
<td>Con</td>
</tr>
<tr>
<td>12ePP (this work)</td>
<td>163</td>
<td>288</td>
</tr>
<tr>
<td>4ePP (this work)</td>
<td>150</td>
<td>279</td>
</tr>
<tr>
<td>4ePP [3]</td>
<td>148</td>
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<tr>
<td>10ePP [13]</td>
<td>134</td>
<td>243</td>
</tr>
<tr>
<td>4ePP [13]</td>
<td>134</td>
<td>-</td>
</tr>
<tr>
<td>IP (this work)</td>
<td>225</td>
<td>233</td>
</tr>
<tr>
<td>IP [28]</td>
<td>314</td>
<td>-</td>
</tr>
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</table>

Table 2.: The energies of the $I_1$ and $I_2$ intrinsic faults for the first-order pyramidal plane computed with DFT and three pseudopotentials, and with an IP generated by Ackland \[28\]. ‘Full’ indicates an unconstrained ionic relaxation allowing atomic displacements parallel and normal to the fault plane. ‘Con’ indicates a constrained ionic relaxation allowing displacements only normal to the fault plane. The energies quoted for the $I_2$ fault with constrained DFT relaxation are for the unstable saddle point configuration in the $\gamma$-surface, which becomes a local minimum with full DFT relaxation. All energies in mJ/m^2.

4. Discussion

To investigate the differences between the 4ePP and the 12ePP $\gamma$-surfaces for the first order pyramidal plane (see Fig. 1(c)) we searched for the smallest nuclear separations in the atomic configurations corresponding to the largest energy differences between the 4ePP and 12ePP results. The largest energy differences occur at $p_1 = [0, 4/11]$ and $p_2 = [1/2, 3/22]$ on the $\gamma$-surfaces. We found the smallest separation with the 4ePP for $p_1$ was 2.58 Å and for $p_2$ it was 2.71 Å, and they occurred at the fault in both cases. These are 0.3 Å and 0.17 Å smaller than the smallest nuclear separation in the perfect crystal. Twice the core radius for the 4 electron pseudopotential is 2.54 Å. Since the wavelength of electrons at 480 eV is 0.56 Å the ‘core radius’ has a finite width of about 0.28 Å. Therefore, when atoms come closer than 2.54 + 0.28 = 2.82 Å the distinction between valence and core electrons begins to break down. Since 2.58 Å and 2.71 Å are less than 2.82 Å this is the likeliest reason for the discrepancies between the 4ePP and 12ePP $\gamma$-surfaces.

It should be noted that the dissociation of a $c + a$ dislocation into two with Burgers vectors $(c + a)/2$ suggested by the $\gamma$-surface line sections of \[1, 2\] is not possible because there is no stable stacking fault at $[0.25, 0.25]$ in the $\gamma$-surface. The translation corresponding to the $c + a = \frac{1}{2}[2113]$ Burgers vector is represented by the centre of the $\gamma$-surface (i.e. $[0.5, 0.5]$) in Fig. 4. If a line section is taken from a corner to the
centre of the $\gamma$-surface a local minimum is found at $\approx [0.2, 0.2]$, as shown in Fig. 6. However, this is not a true minimum, as may be seen in the full $\gamma$-surface in Fig. 4(a).

We have found one low energy stacking fault and one high energy stacking fault in DFT on the first order pyramidal plane. The high energy fault becomes a shallow local minimum only when full, unconstrained relaxation is permitted. It does not appear as a stable fault in the gamma surface, where the only local minimum is at the low energy $I_1$ fault. Because of the high energy of the $I_2$ fault it is unlikely that it will play any significant role in affecting the $\text{c+a}$ dislocation core structure.

![Graph](image)

Figure 6.: A line section of the 4elPP pyramidal $\gamma$-surface shown in Fig. 4(a) along the straight line between [0,0] and [0.5,0.5]. The point [0.5,0.5] on the $\gamma$-surface corresponds to a translation of $\frac{1}{3}[2113]$.

5. Conclusions

The main result of this paper is that we have shown, by calculating the entire $\gamma$-surface for widely spaced (1101) planes in Ti using DFT, that there is just one low energy stacking fault $I_1$ and one high energy stacking fault $I_2$. We obtain energies of 163 and 150 mJ/m$^2$ for $I_1$ and 681 and 700 mJ/m$^2$ for $I_2$ using the 12-electron and 4-electron pseudopotentials respectively. These energies differ from published values by 10–20%, which seems to be about the scatter in published DFT estimates of a range of fault energies.

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References


Appendix A: Convergence tests for \(\gamma\)-surfaces on the basal plane

Using periodic boundary conditions, as described in section 2.2, the intrinsic stacking fault energy (ISFE) on the basal plane was calculated in periodic cells containing \(\{6,10,14,18,22,26\}\) atomic layers using DFT and the IP. The results are shown in Table 3, where it is seen that the cell containing 14 layers yields an ISFE within 2% of those computed using larger cells. This cell size was therefore deemed sufficient. The ISFE is well converged with just 6 layers in the periodic cell when atomic interactions are described by the IP. Interactions between the faults are longer-ranged with DFT.

Table 3.: The ISFE in mJ/m\(^2\) on the basal plane as a function of the number of atomic layers in the periodic cell.

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<thead>
<tr>
<th>Number of layers</th>
<th>DFT ISFE (mJ/m(^2))</th>
<th>IP ISFE (mJ/m(^2))</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>326.9</td>
<td>64.6</td>
</tr>
<tr>
<td>10</td>
<td>314.9</td>
<td>-</td>
</tr>
<tr>
<td>14</td>
<td>306.0</td>
<td>64.5</td>
</tr>
<tr>
<td>18</td>
<td>303.4</td>
<td>-</td>
</tr>
<tr>
<td>22</td>
<td>301.2</td>
<td>64.5</td>
</tr>
<tr>
<td>26</td>
<td>302.7</td>
<td>-</td>
</tr>
</tbody>
</table>

Appendix B: Convergence tests for \(\gamma\)-surfaces on the first order pyramidal plane

To determine the minimum acceptable thickness of the slab for the calculation of the \(\gamma\)-surface using DFT we selected the generalised fault corresponding to the global maximum at \([0,0,0.4]\) of the \(\gamma\)-surface. By varying the thickness of slabs containing this fault we identified the thickness required for the energies of the fault and the two surfaces to be converged. Since this a convergence test for the \(\gamma\)-surface, relaxation displacements were confined to the fault normal. Slab thicknesses ranging from 4 to 16 superplanes (16 to 64 atoms) were considered.

Table 4 lists the reductions in the total energy of slabs that started as slabs of a perfect crystal with no relaxation. For both pseudopotentials a slab of 12 superplanes has a relaxation energy within 2% of the relaxation energies of the two larger slabs.

Fig. 7 shows the interplanar spacings in the \([0,0,0.4]\) generalised fault following the constrained relaxations. There is a large expansion at the fault, and contractions at the two surface layers, with oscillations in the superplane spacing in between. These oscillations decay and almost vanish in the slab with 16 superplanes. The configu-
Table 4.: The relaxation energies in eV of the pyramidal surfaces and an unstable SF for the 4 and 12-electron pseudopotentials in slabs with different numbers of superplanes.

<table>
<thead>
<tr>
<th>Number of Superplanes</th>
<th>12elPP</th>
<th>4elPP</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>1.59</td>
<td>1.56</td>
</tr>
<tr>
<td>6</td>
<td>1.57</td>
<td>1.50</td>
</tr>
<tr>
<td>8</td>
<td>1.67</td>
<td>1.38</td>
</tr>
<tr>
<td>10</td>
<td>1.65</td>
<td>1.32</td>
</tr>
<tr>
<td>12</td>
<td>1.48</td>
<td>1.28</td>
</tr>
<tr>
<td>14</td>
<td>1.47</td>
<td>1.29</td>
</tr>
<tr>
<td>16</td>
<td>1.45</td>
<td>1.26</td>
</tr>
</tbody>
</table>

The relaxations obtained with both pseudopotentials are reasonably well converged with 12 superplanes, particularly with the 12elPP.

Figure 7.: (Colour online) The interplanar spacings through slabs of 8, 12 and 16 superplanes after constrained relaxations. (a) shows the 12elPP results, and (b) shows the 4elPP results.