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Core structure of screw dislocations in hcp Ti: an ab initio DFT study

The core structure of $\frac{\sigma}{3}\langle 11\bar{2}0\rangle$ screw dislocations in α-Ti was studied in the cluster approach with ab initio DFT-GGA, and in both the cluster and quadrupole approaches with a recently highly optimized EAM central force potential. With the EAM potential we have shown that finite-size effects, in the cluster approach, are negligible down to the size studied in the ab initio DFT calculations that have shown unambiguously a preferential prismatic core spreading for the dislocation. Our results are in agreement with previously published approximated calculations using empirical or semi-empirical interaction models: only approximated interaction models, taking explicitly into account the covalent directional bonding of the d electrons, can properly account for the preferential prismatic core spreading against the basal one; and empirical interaction models without angular force components are inadequate. Interestingly, at first sight, the relaxed core structures (basal or prismatic) obtained with empirical or semi-empirical interaction models are almost identical to the ones obtained with the ab initio DFT calculations.

Keywords: Titanium; DFT; EAM; Screw Dislocation; Core Structure

1. Introduction

It has been experimentally shown [1] that plastic deformation in α-titanium is mainly due to the jerky movement of rectilinear $\frac{\alpha}{3}\langle 11\bar{2}0\rangle$ screw dislocations in the prismatic plane. Moreover, light impurities (C, O, N …) have a strong hardening effect with a critical resolved shear stress that decreases rapidly with temperature and presents a discontinuity in its temperature variation associated with a peak in the activation area. Farenc et al. [1] proposed a locking–unlocking mechanism, between a stable sessile and a metastable glissile configuration of the dislocation in the prismatic plane, to explain these specific properties of α-Ti. The validity of this model relies on hypothetical dislocation core structures, dislocation dynamics, and dislocation–impurity interactions, the reality of which can only be established through atomic scale simulations. Such calculations of $T = 0$ K core dislocation structures in α-Ti have yet been performed with approximated empirical and semi-empirical interaction models (see Refs. [2 and 3] and references therein). They aimed to explain why, in hcp metals that all have the same dominant $\langle 11\bar{2}0\rangle$ slip direction, the slip plane is for most of them the basal one but in some cases, like α-Ti, the prismatic one. Legrand [2] has shown that the prismatic glide is related to an increased basal stacking fault energy of transition metals with d fillings between 1.5 and 2.5. This is an effect resulting from the directional d-covalent bonding of partially filled d bands and hence, that cannot be obtained with central force interaction models which always lead to a preferential basal glide [2, 3]. The recent developments in ab initio density functional theory (DFT), as well as the increasing calculation capacities, now allows the study of dislocations at the atomic scale with the much more precise ab initio DFT approach. It opens the possibility of tackling the initially stated problem and at the same time to build up a reliable data base for the construction of good semi-empirical models which are unavoidable for these kinds of studies due to the, nevertheless, very limited size of the systems that can be studied within the DFT approach. We present here such ab initio DFT calculations of the core structure of $\frac{\alpha}{3}\langle 11\bar{2}0\rangle$ screw dislocations in α-Ti. We also performed calculations with a recently highly optimized embedded atom model (EAM) central force potential [4]. It allows us to make size-effect tests and to construct initial pre-relaxed configurations for the ab initio DFT calculations.

2. Methodology

Dislocations are difficult to model because the core is often non-trivial and requires a very accurate atomistic description, whereas a long-range elastic field is also present. Historically, elasticity theory was largely used to model dislocations, ignoring the core. Analytical or semi-analytical approaches, like the Peierls–Nabarro model [5, 6], were developed to take into account the lattice friction and to calculate the dislocation mobility. However, such models are often not sufficient, and an adequate atomistic description of the core has to be made. To model core dislocation structures, the simplest approach, named in this work "Cluster approach", is to use a cylinder periodic along the cylinder axis in which lateral surface atoms are fixed to positions given by the elastic displacement field of the dislocation. However, care must be taken since undesirable effects can arise due to the presence of the surface. A solution to avoid surface effects is to use periodic boundary conditions in all directions. But in that case, one is forced to have a net zero Burgers vector per unit cell. This is generally accomplished by using either a dipole or a quadrupole array of dislocations [7] (named in this work "Quadrupolar approach"). The disadvantage of this approach is the consequent spur-

ious dislocation–dislocation interaction which can be reduced by increasing the distance between the two dislocations of the dipole.

The ab initio DFT calculations were performed with the SIESTA code [8] with a Trouiller-Martins pseudopotential for Ti [9] (3p4s3d valence states) and a PBE-GGA exchange-correlation functional [10]. Localized atomic orbitals have been used with a polarized double-ζ basis set for the 4s electrons and a single-ζ basis set for the 3p and 3d electrons. A Methfessel–Paxton smearing of order 1 was used with an electronic temperature of 100 meV and a mesh cutoff of 400 Ry for the real space grid. For the structural calculations a 7 k-points grid in the irreducible Brillouin zone was used. For all studied systems and methods (EAM or DFT), atoms were relaxed using a conjugate gradient algorithm until convergence of the total energy was reached.

Cluster Approach – The studied systems are of pseudo-hexagonal shape in the direction perpendicular to the dislocation line and are made of 14 atomic planes (EAM) or 2 atomic planes (DFT) parallel to the dislocation line, which are periodically repeated.

Quadrupolar Approach – To construct the system, we followed the approach proposed by Bulatov and Cai [7]. First, starting with a simulation cell equal to a multiple primitive cell in the directions perpendicular to the dislocations line, the dislocation dipole is introduced through the application of the infinite elastic displacement field of the dislocation dipole to the atoms of this cell. The axes of this cell are then tilted in order to suppress the residual mismatch due to the different dipole displacement fields at the borders of the simulation cell, resulting from its finite size. This allows starting the simulation in a well pre-relaxed configuration where only core relaxation effects will occur.

3. Results

Cluster Approach – In this geometry, we first studied, with the EAM potential, the spurious effect of the surface. Different cluster sizes were used: 1078, 1694, 2170, 3108, 4214, and 5488 atoms. The systems were prepared with the atoms positioned according to the linear isotropic elasticity theory [11]. As exemplified in Fig. 1 for the 3108 and 1078 atom systems, where the differential displacement maps (screw component), as defined by Vitek et al. [12], are reported, there is no noticeable difference in the relaxed dislocation core structures.

This result shows that there are no significant effects of the surface on the dislocation core structure, even for the smallest studied hexagon. This is an important result, since this last system corresponds to the 154 atoms system studied later on with the ab initio DFT approach.

The results presented in Fig. 1 were obtained with the initial position 2 of the dislocation line, leading to a basal planar symmetric spreading and a dissociation into two Shockley partials. We then studied the effect of the initial position of the dislocation line on the core structure, first with the EAM potential with the 3108 atoms system (Fig. 1), and then with the ab initio DFT method with the 154 atoms system.

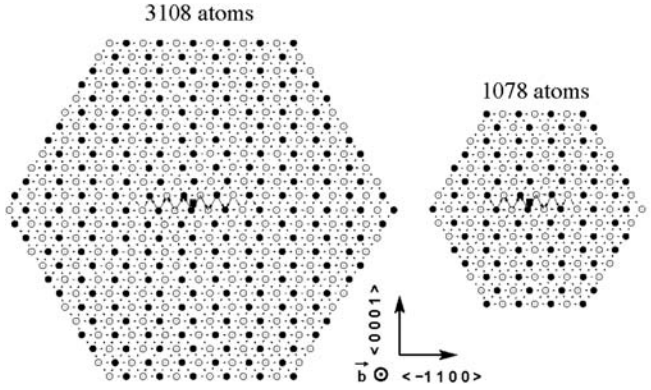
In the EAM case, depending on the initial position of the dislocation center, two final core structures are obtained (Fig. 2): one into the basal plane (initial positions 1, 2, and 5) as described previously for position 2 with a 608 ± 1 meV Å^{-1} excess energy (Table 1) and the other into the prismatic plane (initial positions 3, 4, and 6) with a 634 ± 1 meV Å^{-1} excess energy (Table 1). In the prismatic case the dislocation core is non-planar: it spreads mainly in the prismatic plane but with large secondary spreading components out of the prismatic plane.

Since all these structures have the same number of atoms, the excess energy difference between the basal and the prismatic configurations is a very good approximation of the energy difference between the corresponding dislocation cores. The slightly lower excess energies of the basal configurations show that the EAM central-force potential favors the basal spreading instead of the experimentally observed prismatic one.

Three initial positions (2, 3, and 5 in Fig. 1), leading to either basal or prismatic spreading with the EAM potential, were chosen to study the dislocation core with the ab initio DFT approach. Contrary to what was observed with the EAM central force potential, a prismatic core spreading (Fig. 2), very similar to the ones obtained with the EAM potential, was observed in all three cases. Initial positions 2 and 5 lead certainly to the same final structure (they differ by a 180° rotation around the dislocation axis). Their small structure and energy differences probably arise from their

Table 1. Excess energies (meV Å^{-1}), defined as the energy difference between the cluster with the dislocation and without it ($E_{\text{disloc}} - E_{\text{cluster}}$), of the different core structures before and after relaxation with the EAM central force potential.

Initial Position	Core Structure	before relaxation	after relaxation
1/2/5	Basal	807.5/826.4/826.1	608 ± 1
3/4/6	Prismatic	823.9/823.0/842.1	634 ± 1



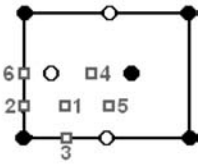


Fig. 1. Comparison of the relaxed dislocation core structures (screw component) with systems of different sizes with the EAM potential. Black and empty circles denote atoms belonging to different planes. Black square: initial position of the dislocation line. Gray squares: different initial positions of the dislocation line in the unit cell of hcp Ti.

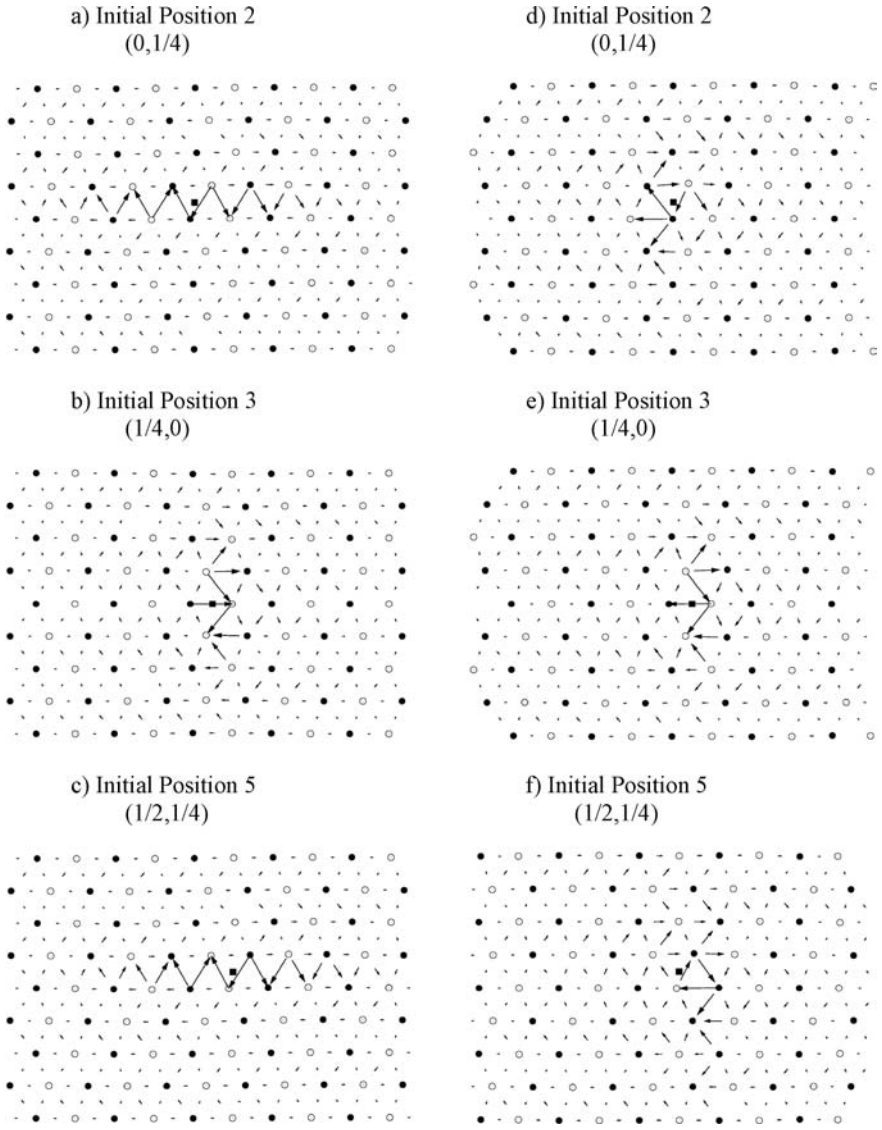


Fig. 2. Differential displacement maps (screw component) for three initial positions (depicted as black squares) with the EAM potential (a, b, c) and with the DFT method (d, e, f). In brackets are given crystallographic coordinates in the cell of the plane $\langle 11\bar{2}0 \rangle$ as shown in Fig. 1.

slightly different positions relative to the surface and subsequent interaction [13]. This is also consistent with their equivalent structures in the cell in the translation exchanging the two planes (black and empty dots in Fig. 1) confirming the very small influence of the surface despite the small size of the simulation cell. The final structure of position 3 is also very similar to the final structures of positions 2 and 5, however its excess energy is certainly too different from those of positions 2 and 5 to only result from surface effects. Indeed its position in the cell is very different from positions 2 and 5 which could explain that energy difference.

In order to force a basal spreading we took, as initial configurations, two of the basally-relaxed configurations obtained with the EAM potential (relaxed configurations 2 and 5 of Fig. 2). Whereas the core structure remains in the basal plane in the case of the pre-relaxed configuration 2, the geometry of the dislocation core is quite changed by the relaxation in the case of pre-relaxed configuration 5, leading to a highly non-planar core. The excess energies of the studied relaxed configurations are reported in Table 2. Contrary to the EAM case and in agreement with experiments the prismatic cores have the lower excess energies.

Quadrupolar Approach – Two initial positions were selected for the quadrupolar study with the EAM potentials: positions 1 and 3 leading, in the cluster approach, to the basal and the prismatic spreadings, respectively. Six different distances between the dipole dislocations were studied: 20, 40, 60, 80, 100, and 125 Å (i.e. 4, 8, 12, 16, 20, and 25 unit Ti cells) corresponding to 896, 3584, 8064, 14 336, 22 400, and 35 000 atoms, respectively.

For system 1 (basal) we observe an annihilation of the dipole until 125 Å (i.e. 25 unit cells), whereas for system 3 (prismatic) at distances larger than 8 unit cells the dipole is stable and the final relaxed core structures are similar to the ones obtained in the cluster approach. When annihilation occurs it always proceeds through basal glide. To ensure that the rectangular form of our system implies no artifacts, a square system in which the distance between the

Table 2. Relaxed excess energies (meV $Å^{-1}$) of the different core structures, using ab initio DFT.

Initial Position	Core Structure	After relaxation
2/5	Prismatic	472.1/461.8
3	Prismatic	415.5
2 (EAM pre-relaxed)	Basal	502.9
5 (EAM pre-relaxed)	Non-planar	466.9

Table 3. Stacking fault excess energies (γ_{I1}, γ_{I2}, γ_{IE}) and γ_{prism} for hcp Ti, in mJ m^{-2}. (a) this work, (b) Ref. [3]: BO (Bond-order potential), (c) Ref. [2] (Tight Binding), (d) Ref. [14], (e) Ref. [15] and (f) Ref. [16].

	EAM[a]	EAM[b]	BO[b]	TB[c]	DFT[a]	Exp.
γ_{I1} (AB|CB)	31				150	
γ_{I2} (AB|CA)	54	64	110	370(290)	260	290[d], 300[e]
γ_{IE} (AB|C|AB)	82				354	
γ_{prism}	365	253	260	140(110)	233	150[f]

two dislocations of the dipole is the same in the basal and in the prismatic directions, was also studied: there is no significant change in the observed results.

The preliminary results obtained with this "quadrupolar approach" are perfectly coherent with those obtained with the "cluster approach". If this is confirmed by the complete quadrupolar study, which is currently under progress, it will give a high degree of confidence to our results and it will help for a precise evaluation of the core energies and later-on of the Peierls barriers.

4. Discussion – conclusion

Accurate DFT calculations of the $\frac{\alpha}{3}\langle 11\bar{2}0\rangle$ screw dislocations core structures in α-Ti have shown that the prismatic dislocation spreading is favored over the basal one in agreement with experimental observations, whereas the approximated EAM central-force interaction model predicts a preferred basal spreading. These results confirm previous calculations with approximated interaction models [2, 3]: only interaction models taking explicitly into account the covalent directional bonding of the d electrons can properly account for the preferential prismatic spreading. Empirical interaction models without angular force components (central-force models) are inadequate.

As initially demonstrated by Legrand [2] this result can be correlated with the systematic under-evaluation of the basal stacking fault energy by central force interaction models (Table 3), favoring a basal dissociated dislocation against a prismatic spreading.

From our DFT calculations we cannot yet extract values for the dislocation core energies, however we can evaluate the difference in core excess energies between the basal and the prismatic cores which is ≈ 87 meV Å^{-1} to be compared to ≈ 25 meV Å^{-1} in the TB scheme [2] or with the BO potential [3]. A difference which is certainly significant if one takes into account the very different values obtained for the stacking-fault energies (Table 3).

Interestingly, at first sight, the relaxed core structures (basal or prismatic) obtained with empirical or semi-empirical interaction models taking into account the angular character of the bonds are almost identical to the ones obtained in the ab initio DFT calculations. If confirmed by a more detailed analysis of the core structures, this is a very important result since it means that semi-empirical approaches similar to the ones used in references [2] (TB) and [3] (BO) are reliable approximations for studying dislocations in α-Ti. However the energetic analysis reveals that from the energetic point of view they need to be improved. The determination of the core dislocation structure is the initial step towards a theoretical description of the peculiar plastic deformation mechanism in α-Ti described in the introduction. The next step is now to look at dynamical parameters like the Peierls barriers.

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