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AB-INITIO SIMULATION OF a/2<110> SCREW DISLOCATIONS γ-TiAl

C. Woodward and S.I. Rao

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Pamela M. Schaefer
Principal Materials Engineer
Technical & Strategic Planning Office
Materials and Manufacturing Directorate

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C. Woodward (Northwestern University)
S.I. Rao (UES, Inc.)

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2225 North Campus Drive
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By Authors:

C. Woodward[+,*] and S.I. Rao*
*Materials and Processing Division
UES, Inc., Dayton, OH
[+]Department of Materials Science and Engineering
Northwestern University, Evanston, IL

Contact Author:

Chris Woodward
Department of Materials Science and Engineering
2225 North Campus Drive
Northwestern University, Evanston, IL 60208-3108 USA
c-woodward@northwestern.edu
847-491-2232
847-491-7820 (FAX)

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C. Woodward[+,*] and S.I. Rao*

Air Force Research Laboratory

Materials and Manufacturing Directorate

*Materials and Processing Division

UES, Inc., Dayton, OH

[+]Department of Materials Science and Engineering

Northwestern University, Evanston, IL

Abstract

The equilibrium core structure of an isolated a/2<110]{111} screw dislocations is calculated using a first-principles pseudopotential-planewave method within the Local Density Approximation of Density Functional Theory. In this work the local dislocation strain field is self-consistently coupled to the long-range elastic field using a flexible boundary condition method. This ab-initio adaptation of the Greens Function Boundary Condition method makes it possible to simulate the dislocation in a very small periodic cell without compromising the fidelity of the final core configuration. Supercells of 210, 288 and 420 atoms are used to evaluate the local screw and edge displacements of a straight a/2<110]{111} screw dislocation in γ-TiAl. The predicted dislocation core is non-planar with significant portions of the dislocation core spread on conjugate {111} glide planes. By applying a pure (111) shear stress the lattice friction stress is estimated

to be approximately 0.006μ in reasonable agreement with experimental observations. The non-planar character of the dislocation core suggests that the dislocation is sessile, and would readily glide on either of two {111} slip planes. The dislocation core also produces small but significant edge components that are expected to interact strongly with non-glide (e.g. Escaig) stresses producing significant non-Schmid behavior.

1. Introduction

Alloys based on the $L1_0$ phase of titanium-aluminum (γ-TiAl) are promising candidates for aerospace applications due to their superior high temperature strength, oxidation resistance and low density. These alloys also exhibit an increasing yield stress with increasing temperature in the temperature range of 873-1073 K (Kawabata, Kanai, and Izumi, 1985). This anomalous yield stress is analogous to that observed in several other intermetallic alloys such as Ni_3Al and Ni_3Ga. In TiAl the deformation behavior is quite complex, and often involves the simultaneous operation of multiple slip systems (<011]{111}, ½<112]{111} and ½<110]{111}). There has been considerable interest in characterizing the temperature dependent flow behavior of each slip system using experimental and computational methods. Recently considerable attention has been focused on the role of ½<110]{111} ordinary screw dislocations in producing this high temperature strengthening.

The anomalous yield stress in γ-TiAl was originally reported by Kawabata et al. (1985) for single crystal Ti-56Al alloys . In alloys such as TiAl, where the material remains ordered up to its melting temperature the enhanced strengthening is associated with the formation of thermally activated dislocation glide barriers. While specific details of the dislocation blocking mechanism remain controversial it is generally accepted that the dislocation core structure is the source of the enhanced yield stress in both the $L1_2$ (Ni_3Al, Ni_3Ga) and $L1_0$ (TiAl) alloys. Based on TEM observations several groups have proposed dislocation barriers based on the ½<110]{111} screw dislocations. Louchet and Viguier proposed that the TiAl lattice produces Peierls-type lattice friction stress, similar

to the bcc transition metals, and that the ordinary screw dislocations move by a kink-pair mechanism (Louchet and Viguier, 1995). Assuming that the dislocations cross-slip quite easily Louchet and Viguier suggested that pinning points are formed when kinks on different {111} planes collide. The density of these pinning points increases with temperature making the dislocation immobile. Using TEM observations Sriram and co-workers observe a dislocation substructure more consistent with dislocation glide involving frequent double cross slip (Sriram, Dimiduk, Hazzledine and Vasudevan, 1997). The resulting jog formation produces a large glide resistance on the dislocation, and the density of these jog segments increases with temperature. Both of these models require that the ordinary screw dislocation will easily cross-slip, and that the lattice friction stress is large enough to favor movement by kink-pair formation.

In this paper we calculate the equilibrium core structure of an isolated ½<110]{111} screw dislocation in TiAl using an ab-initio method. This work is motivated by the dislocation core structures predicted for the BCC transition metals, where non-planar dislocations are thought to produce large lattice friction stresses and significant non-Schmid effects (see for example Taylor, 1992). Atomistic and first principles calculations have shown that in the some BCC metals straight dislocations readily cross slip, in a manner consistent with wavy slip lines, or pencil glide (Woodward and Rao, 2001, Woodward and Rao, 2002, Ito and Vitek, 2001, Yang, Soderlind and Moriarty, 2001). The propensity for cross-slip in both TiAl and the BCC metals is thought to be related to the shape of the local dislocation strain field (the dislocation core). Also at low temperatures both material systems have high relative Peierls stresses and show a

strongly decreasing yield stress with increasing temperature consistent with kink-pair mediated glide (Dimiduk, Rao, Partharasarthy and Woodward, 1991).

Several groups have studied deformation modes in TiAl using atomistic methods based on Embedded Atom method (EAM). We have studied the core structure and mobility of ordinary and super-dislocations using parametric EAM potentials fit to a range of planar fault energies (Simmons, Rao and Dimiduk, 1997, Rao, Simmons, Woodward and Dimiduk, 1995). As in simple fcc metals the deformation modes in TiAl can reduce their elastic energy by dissociating and forming smaller partial burgers vectors separated by a planar fault. The equilibrium configuration balances the repulsive interaction of the partial dislocations against the energy cost of extending the planar fault that lies between the two partials. In TiAl the crystal can sample a wider variety of planar faults (stacking fault, and anti-phase boundary or a complex stacking fault) and can sustain dislocations with larger burgers vectors (e.g. super-dislocations). Therefore, it is not surprising that the dislocation core geometries predicted using atomistic potentials strongly depends on how the atomistic potentials are constructed and the value of the planar fault energies produced by the potentials. Also, Simmons et al. 1997 have shown that the predicted lattice friction stress is strongly dependent on the assumed stacking fault energies.

In this study we avoid the complications imposed by empirical potentials by directly calculating the equilibrium configuration using an ab-initio method. Recently we have developed a first-principles flexible-boundary method that self-consistently couples the local strain field of the dislocation core to the long-range elastic field. The First

Principles Greens Function Boundary Condition (FP-GFBC) method has been used in studies of the equilibrium dislocation strain-field and lattice friction stress of ½<111> screw dislocations in bcc Mo and Ta (Woodward and Rao, 2002, 2001). The flexible boundary condition method has also been used with atomistic potentials to study 2 and 3 dimensional dislocation defect structures in transition bbc and fcc metals and intermetallics (Rao et al. 1998, 1999).

As early as 1970 Basinski and co-workers were studying the equilibrium core structure and the lattice friction stress of bcc metals using an effective ion-ion potential generated from a fundamental electronic structure theory (Basinski, Duesbery, Pogany, and Taylor, 1970, Basinski, Duesbury and Taylor, 1971). The potentials, based on the one-orthogonalized plane wave bare electron–ion matrix and an electron screening function, were used to model second-row free-electron metals such as sodium. While these early techniques were not capable of simulating the more complex electron scattering behavior of the bcc transition metals they did clearly illustrate the scope of behavior one could expect from dislocations in the bcc lattice. We have recently studied the ½<111> screw dislocations in the group VA and VIA transition metals (Mo and Ta) using a current first principles method and found: significant core spreading on conjugate (110) planes, highly anisotropic Peierls stress, and dislocation movement by displacement on alternative {110} planes (Woodward and Rao, 2001, Woodward and Rao, 2002). Surprisingly, many of these results were first observed in bcc sodium by Basinski and co-workers using an effective ion potential calculated from first principles methods.

This paper is in the same spirit as the original papers by Basinski (1970, 1971) as we try to apply the most robust methods to enhance our understanding of plastic deformation. Plasticity is more complex in TiAl by virtue of the fact that it is an intermetallic and has more active slip systems than the bcc metals. However, the general principles applied in the earlier work can also be applied here. We are interested in what dislocation core geometries the lattice produces, how these cores are affected by glide and non-glide stress and the resulting lattice friction stress. In this paper we present preliminary results of an ongoing study of deformation modes in TiAl and current lattice friction results are limited to pure shear stress on the (111) plane.

2. Computational Methods

2.1 Electronic Structure Calculations

The calculations have been performed using the ab-initio total-energy and molecular-dynamics program VASP (Vienna Ab-initio Simulation Package) developed at the Institut fur Theoretische Physik of the Technische Universitat Wien (Kresse and Hafner, 1993, Kresse and Hafner, 1994, Kresse and Furthmueller, 1996, Kresse and Furthmueller, 1996). The VASP electronic structure and lattice statics optimization procedures have proven to be very robust. We have optimized dislocation core structures in the bcc transition metals using cell sizes up to ~1000 atoms on current parallel supercomputers (e.g. COMPAQ GS40). In TiAl we found that a cell size of 288 atoms was sufficient when the GFBC method was properly implemented. The supercell calculations described here are performed with 4 special k points with ultra-soft pseudo-potentials for Ti and Al (Vanderbilt, 1990, Kresse and Hafner, 1994). These pseudo-

potentials give reasonable lattice parameters and elastic constants (Table 1) when compared to experiment and previous electronic structure calculations. Lattice Greens Function parameters for Ti and Al were derived with the VASP formalism using the methods described in Rao, et al., 1998.

2.2 Computational Details

The electronic structure method uses a supercell approximation which requires periodic symmetry along the three lattice directions. Unfortunately, the symmetry of a single dislocation only allows periodicity along the dislocation line. In previous applications of the FP-GFBC method we have illustrated several approaches to circumvent this problem (Woodward and Rao, 2002, 2001). In the calculations presented here we employ a domain boundary to truncate the simulation cell parallel to the dislocation line (Figure 1). The supercell walls normal to $<1\,\bar{1}\,2]$ and $<1\,\bar{1}\,\bar{1}]$ directions can be considered as domain boundaries. The supercell size and geometry is chosen to minimize the overlap of atomic charge densities in the domain boundary while maintaining the correct lattice parameters and atomic density. In principle if several atoms are in close proximity the electronic structure calculation will fail, or produce significant changes in the local charge density (e.g. charge dipoles). In these calculations the nearest neighbor distance for atoms across the domain boundaries atoms is always greater than 90% of the bulk nearest neighbor distance. The charge dipoles produced at the domain boundary produce very small perturbations in the charge density when compared to the charge dipole found at a metal surface.

The isolated straight a/2<110] screw dislocation is simulated using a cell with lattice vectors $i<1\bar{1}2]/2$, $j<1\bar{1}\bar{1}]$, $k<110]/2$. Table 2 lists the cell parameters in terms of i, j and k and the radius used for regions 1 and 2 as shown in Figure 1b. The a/2<110] screw dislocation was introduced into the simulation cell by displacing all atoms according to anisotropic elasticity theory calculated using Stroh's sextic formalism (Stroh, 1958). Since the anisotropic elasticity solution diverges at the origin, the displacement field was centered between atomic positions. This set of atomic positions was then optimized using the Hellmann-Feynman forces and the FP-GFBC method, which has been described previously (Woodward and Rao, 2002, 2001). The atomic forces were converged so that the average force on an atom within regions 1 and 2 was less than 0.005 eV/Å. The GFBC method is described briefly in the next section.

2.3 Green's Function Boundary Conditions

The simulations presented in this paper include systems with periodic symmetry along the dislocation axis. We have previously described flexible boundary condition methods for both 2- and 3-D atomistic systems based on the lattice-Greens Function method (Rao et al., 1998). In 2-D simulation cells, the incompatibility forces that build up at the boundary between regions 1 and 2 (see figure 1) are relieved by displacing all the atoms within the simulation cell according to the GF solution,

$$u_i^m = \sum_{j,n} G_{ij}^{mn}(R_{mn}) f_j^n \qquad (1)$$

where the indices m, n denote atoms, the indices i, j denote the Cartesian components, and $R_{mn} = R_n - R_m$. When $R_{mn} > R_0$, the elastic Green's function (GF) of the perfect lattice, appropriate for line forces, is used as an approximation to G_{kj}^{mn} (Stroh, 1962,

Bacon, Barnett and Scatergood, 1979). Since the elastic GF diverges at short distances ($R_{mn} < R_0$) the lattice GF of the perfect lattice is used as an approximation to **G**. The lattice GF of the perfect lattice is calculated using a simple numerical procedure described by Rao *et al.* 1998. In atomistic applications of the GFBC method it was found that a value of 0.50nm for R_0 was sufficient (i.e. the solutions of the elastic and lattice Greens Functions match) for the TiAl EAM potential (Rao, 1999). In the derivation of this first principles lattice Greens Function we find the convergence to the elastic Greens function at a comparable distance. Because the Greens functions are that of a perfect lattice and the simulation cell contains an a/2<110] screw dislocation, the atomistic optimization procedure must iterate between optimizing forces in regions 1 and 2 until all the forces are completely relaxed. In the first principles adaptation of the Greens Function Boundary Condition method the atoms are moved according to the Hellmann-Feynman forces which are derived at every step of the procedure.

3. Results

3.1 Planar fault energies

From our previous work using parametric EAM potentials we expect the dislocation core structure will be sensitive to the scale of the planar fault energies predicted by the first principles plane wave method. Therefore, before proceeding with calculations on the dislocation core itself we calculated the planar faults predicted by the first principles method, these results are shown in Table 3. In these calculations we relaxed the atomic positions using the Hellmann-Feynman forces, however the predictions are still for

stoichiometric TiAl at 0K. The results are within the scatter found using other first principles methods, but are somewhat larger than that observed experimentally using weak beam TEM (Hug, Loiseau and Veyssiere, 1988, Woodward, MacLaren and Rao, 1992). The range of experimental values given in Table 3 for the Complex Stacking Fault (CSF) energy is the result of fitting high resolution TEM images of a ½<110] mixed dislocation to dislocation strain fields produced by parametric EAM potentials (Simmons, Mills and Rao, 1997). The CSF energy has not been determined using conventional weak beam TEM because the distance between the Shockley partials bounding the planar fault is beyond the resolution of these methods. The predicted CSF energies are consistently lower than that suggested by a parametric fit to high resolution TEM images.

3.2 Equilibrium dislocation cores

The ½<110] screw dislocation was relaxed from several elastic centers as defined by the anisotropic elasticity theory. The resulting equilibrium core structures for simulations using 288 and 420 atom unit cells are shown using differential displacement plots in Figures 2 and 3 (Vitek et al., 1970). In these figures the relative atomic displacements near the dislocation core are represented by a vector placed between the two atoms. In Figure 2, which shows the screw displacements, the length of the vectors are normalized to the magnitude of the burgers vector. In Figure 3, which shows the edge components, the lengths of the vectors are scaled by a magnification factor (x5) so that the edge components can be visualized. The results for the 288 atom (R_2~16.0 A) and 420 atom (R_2~19.8 A) cells are very similar. The FP-GFBC method appears to be well converged as a function of cell size for cells of 288 atoms. In the smallest simulation cell (R_1~7.1 A, R_2~12.6 A) we found some non-linear interaction of the dislocation core between regions

1 and 2 indicating that the cell was too small to contain the dislocation core. The charge density near the dislocation core is shown in Figure 4. The isosurface charge-density plot shows the charge density looking down the dislocation line (the screw direction) using the same coordinate system as the differential displacement plots shown in Figure 2. We also include two insets showing the charge density in the all Ti and all Al (001) planes near the dislocation core. The upper inset shows the Ti atoms in an inclined row consistent with the presence of a screw dislocation. Also, there is charge buildup between nearest neighbor Ti atoms, consistent with the nearest neighbor bonding found in bulk TiAl. In the lower inset there is a large screw (<110]) displacement in the all Al plane near the center of the dislocation core, in the differential displacement plots this is represented by the large vector between the two Al atoms adjacent to the core.

3.3 Applying stress

In order to estimate the lattice friction stress we have applied a pure shear stress in the $(1\bar{1}\bar{1})$ plane to a 288 atom simulation cell containing an a/2<110] screw dislocation. Preliminary estimates are that the dislocation will glide on the (111) plane in response to a pure shear stress of approximately 0.006μ. The motion of the dislocation is illustrated (Figure 5) in a series of differential displacement plots for a dislocation moving on the $(1\bar{1}\bar{1})$ plane.

4. Discussion

We illustrate in Figure 6 the variety of dislocation core structures found for the ½<110]{111} screw dislocation using atomistic potentials (Simmons et al., 1997, Girshick and Vitek, 1995). These studies produced dislocation configurations ranging

from a planar core with extended partial dislocations to a very compact core with significant screw displacements on several glide planes. Several studies also found meta-stable configurations that transformed to planar configurations under stress. The variation in dislocation core structure is directly related to the structural parameters the potentials are fit to and the resulting planar fault energies produced by the potentials. If the complex stacking fault energy (γ_{CSF}) is low enough the ordinary screw dislocation will dissociate into two 1/6<112] type partials separated by a CSF. As the fault energy increases the dislocation become more compact. When γ_{CSF} is large enough the core takes on a non-planar configuration analogous to that found in the BCC transition metals. Also, Simmons et al. 1997 found that the lattice friction stress increased with increasing γ_{CSF}, presumably because of the variation in core geometry.

The plane-wave pseudo-potential method gives a γ_{CSF} of 372 mJ/m^2. We expect the equilibrium core structure produced by the FP-GFBC method to be similar to the dislocation core found by Simmons et al. using an atomistic potential with γ_{CSF} equal to 320 mJ/m^2 (see Figure 6). Using the FP-GFBC method we have not found a planar ½<110] core, though it is possible that such a core could be produced by sampling a wider range of elastic centers. Also, surprisingly the atomistic core structure most like the first principles results is the non-planar core produced by Girshick and Vitek, 1996 using atomistic potential with γ_{CSF} equal to 275 mJ/m^2. These cores have a large screw displacement of a pair of Al atoms adjacent to the center of the dislocation core and almost symmetric distribution of the strain field on the $(1\,\bar{1}\,\bar{1})$ and $(\bar{1}\,1\,\bar{1})$ planes.

As a pure (111) stress is applied the dislocation begins to distort with the displacements extending asymmetrically along the (111) planes. As the dislocation goes over the Peierls barrier (Figure 5c) there continues to be significant extension of the core on the $(\bar{1}\,1\,\bar{1})$ cross slip plane. Because the core is spread over several glide planes it is difficult to characterize the core as planar as the dislocation is moving on the glide plane. The concentration of strain on the cross-slip plane implies that the dislocation can easily cross slip. Also, from Figure 3 we note that there are small but significant edge displacements near the dislocation core. These displacements will strongly couple to non-glide stresses, such as an Escaig stress, and will produce significant non-Schmid effects (Duesbery and Vitek, 1998, Escaig, 1968). The edge displacements seen here are approximately 3 times larger than those predicted in bcc Mo and Ta (Woodward and Rao, 2001).

5. Summary

We have calculated the equilibrium dislocation strain field of a ½<110]{111} screw dislocation in γ-TiAl using an electronic structure method based on the Local Density Approximation of Density Functional Theory. A flexible boundary condition method was used to isolate a single dislocation in the ab-initio supercell calculation. Here the method employed lattice Greens functions for a binary system, TiAl, which were derived using a simple, well defined procedure. FP-GFBC iterative method converged rapidly with cell size and was relatively straightforward to implement for the $L1_0$ lattice.

The ½<110] screw dislocation is predicted to be non-planar, with significant spreading onto two {111} planes. This dislocation core configuration is expected to cross slip easily.

Also, the dislocation core produces small but important edge displacements that can produce significant non-Schmid behavior. While the predicted lattice friction stress, ~ 0.006μ, is large for an FCC metal it is consistent with the high strength expected for these alloys. Current AYS models based on the ordinary screw dislocation have two fundamental requirements: a high Peierls stress and easy cross slip. The current results strongly suggest that these requirements are satisfied in γ-TiAl.

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Tables

Table 1

Lattice and elastic parameters for γ-TiAl. The lattice constants are given in Angstrom and the elastic constants in Mbar.

Method	a_0(A)	c/a_0	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}
FLAPW[1]	3.946	1.01	1.90	1.05	0.90	1.85	1.20	0.50
FLAPW[2]	3.90	1.04	1.88	0.98	0.96	1.90	1.26	1.00
NCPP[3]	3.959	1.026	1.71	0.96	0.91	1.75	1.11	0.84
VASP	3.9197	1.022	1.79	0.97	0.97	1.77	1.25	0.72
Exp.[4]	4.005	1.016	1.86	0.72	0.74	1.76	1.01	0.77

[1] From Fu and Yoo, 1991.

[2] From Mehl et al., 1991.

[3] From Woodward and Kajihara, 1998.

[4] From He et al., 1995.

Table 2

Scale of Lattice vectors (see text) and size of lattice GFBC regions, given in Angstroms.

Total number				Region 1		Region 2	
of atoms	i	j	k	R_1	# of atoms	R_2	# of atoms
210	7	5	1	7.212	31	12.62	95
288	8	6	1	9.779	55	16.03	145
420	10	7	1	13.70	103	19.81	223

Table 3

Planar Fault Energies

Method	SISF	(111)APB	CSF
FLAPW[a]	90	560	410
FLAPW[b]	172	667	363
FP-LMTO[c]	134	710	314
VASP	160	610	372
Exp.[d]	140	250	470-620[e]

[a] From Fu and Yoo, 1997

[b] From Ehmann et al., 1998

[c] From Vitek et al., 1997.

[d] From Woodward et al., 1992.

[e] From Simmons et al., 1997

Figure Captions

Fig. 1. Schematic diagram of the supercell used to simulate an isolated dislocation in g-TiAl. The shaded regions on the edge of the cell represent domain boundaries (see text).

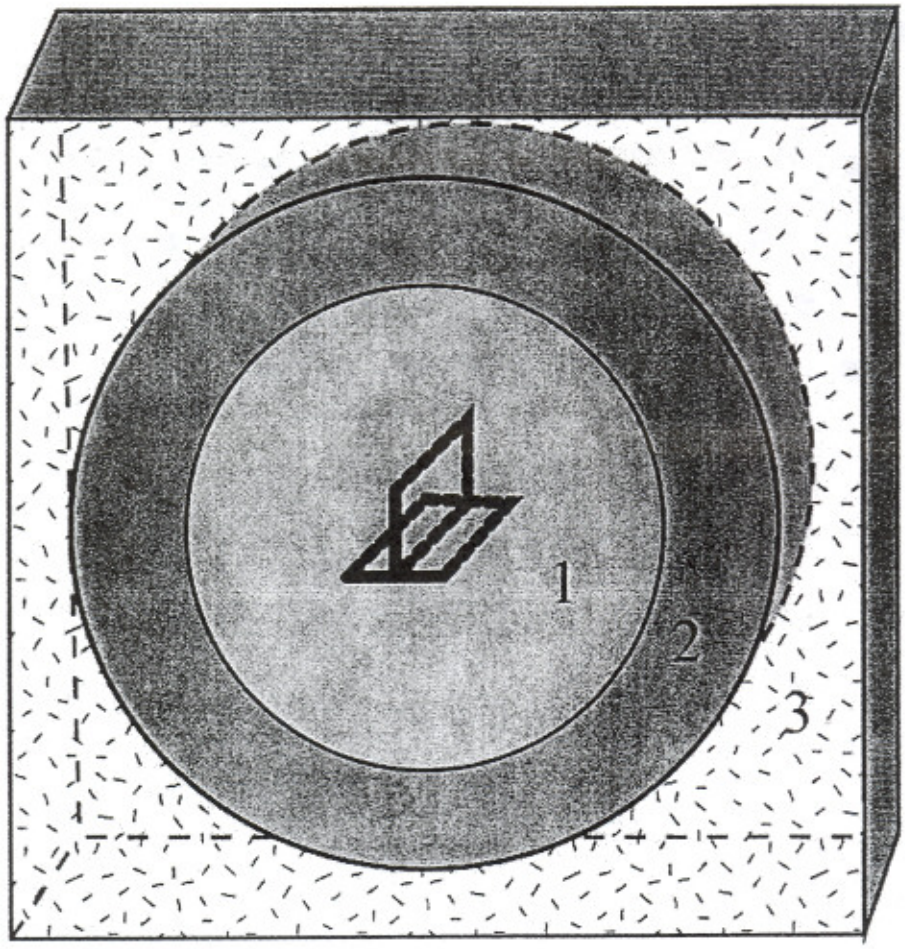
Fig. 2. Differential Displacement plots showing the screw components of the predicted equilibrium dislocations core for ½<110] screw dislocations in TiAl for cells containing a) 288 atoms and b) 420 atoms. The open and filled circles represent the positions of Al and Ti atoms respectively.

Fig. 3. Differential Displacement plots showing the edge components of the predicted equilibrium dislocations core for ½<110] screw dislocations in TiAl for cells containing a) 288 atoms and b) 420 atoms.

Fig. 4. Charge density iso-surface plot of the a/2<110] screw dislocation in γ-TiAl. The insets show the cross section of the charge density in the all Ti and all Al {001} planes near the core region. Note the large displacement of Al atoms in the screw direction shown in the lower inset.

Fig. 5. Differential displacement plots of a ½<110] screw dislocation moving under a pure (111) glide stress.

Fig. 6. Differential displacement plots showing the dislocation core geometries for an a/2<110] screw dislocation in γ-TiAl derived using atomistic potentials with different values of the complex stacking fault energy (mJ/m^2). ([a]From Simmons et al. 1997 and [b]from Girshick and Vitek, 1996.)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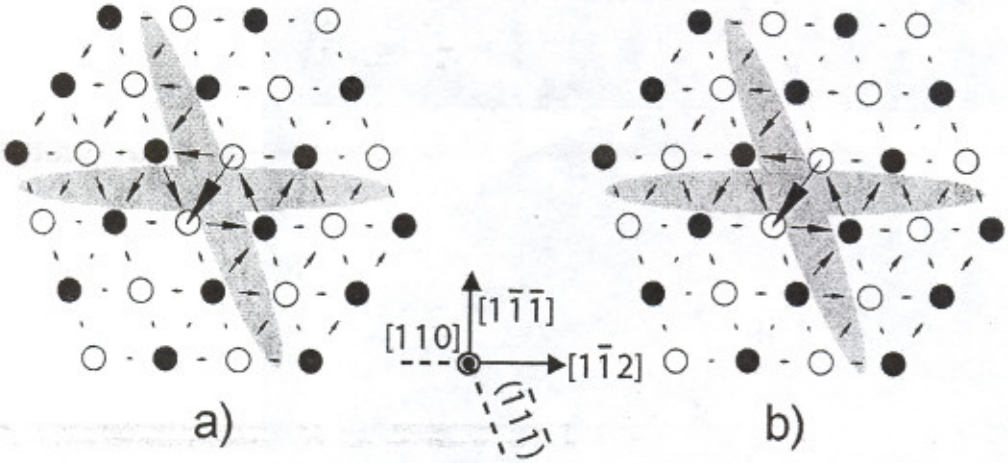
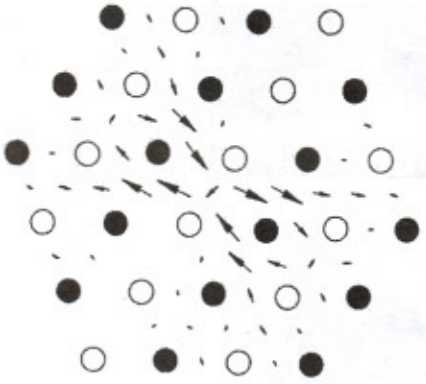
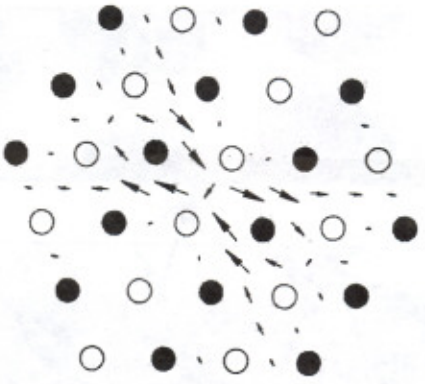
2
3


[1 1̄ 1̄]
[1 1 0]
[1 1̄ 2]
(1̄ 1 1)
a)
b)



a)



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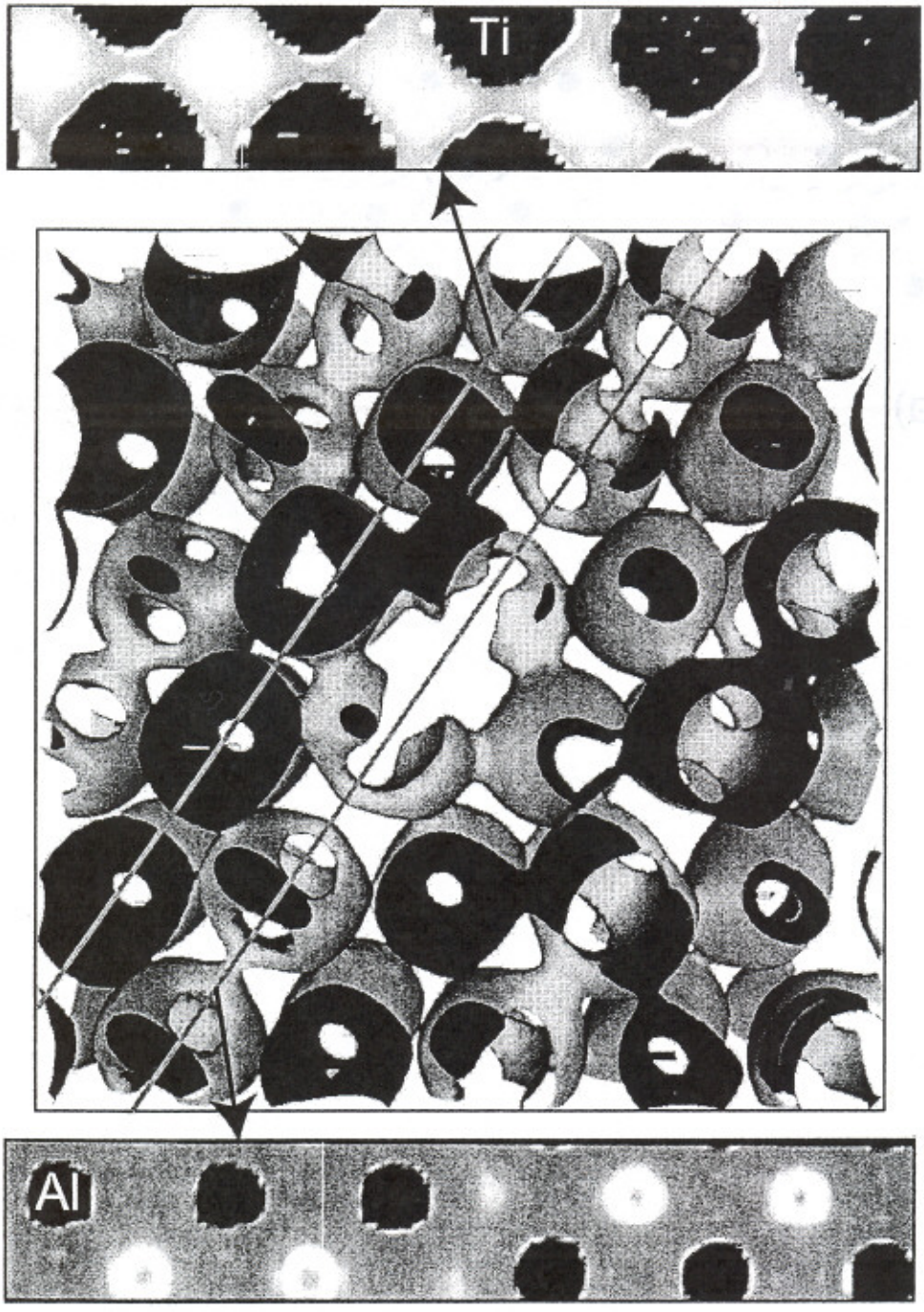
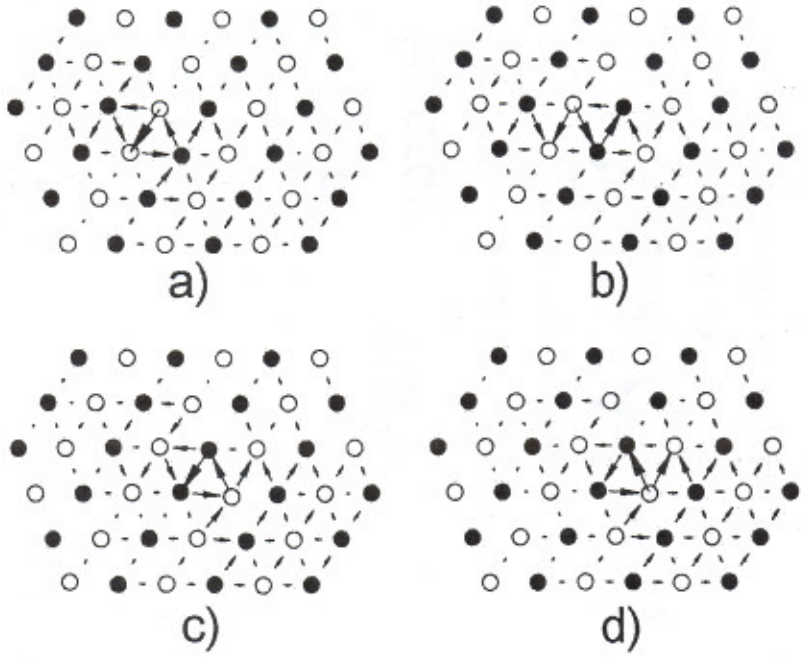
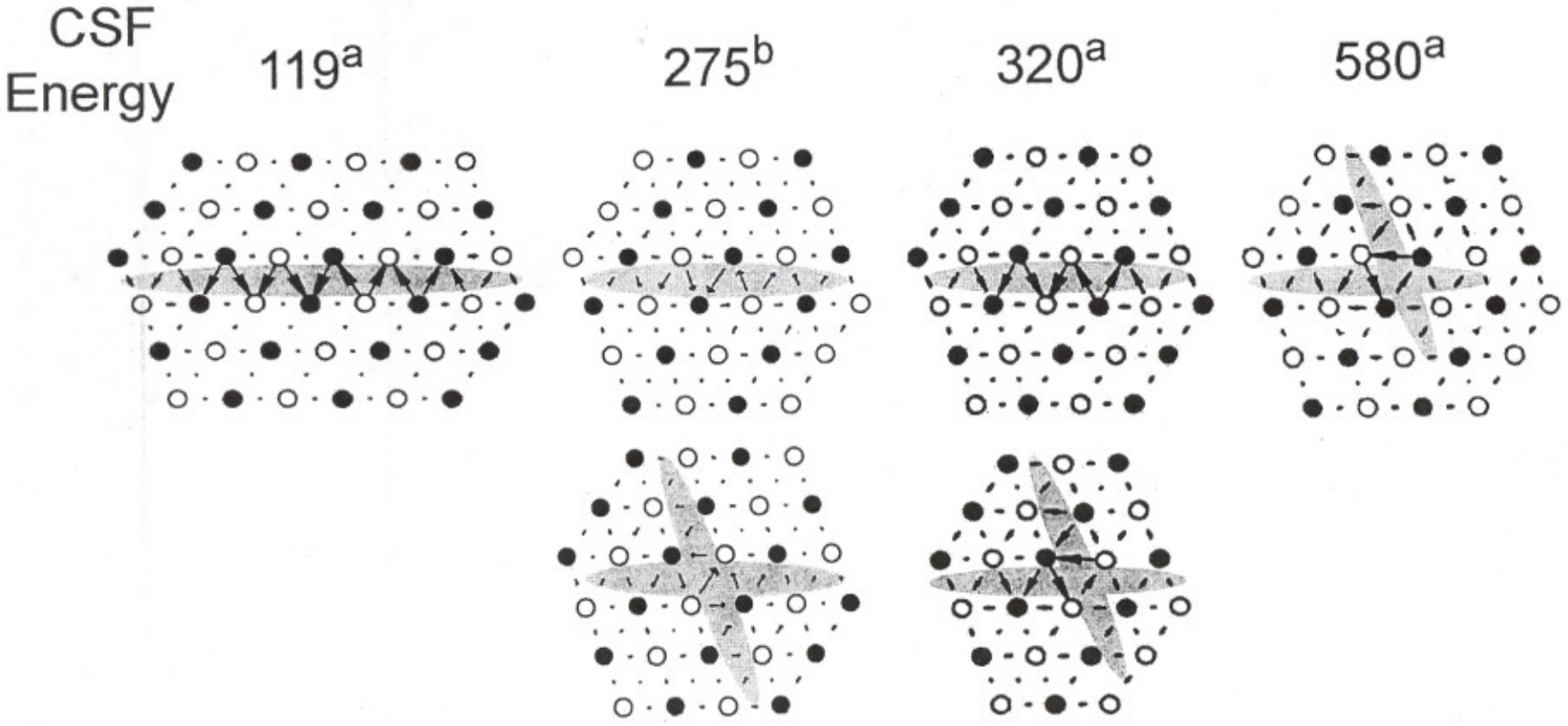

Ti
Al


a)
b)
c)
d)


CSF
Energy
119a
275b
320a
580a