

ATOMIC LEVEL MODELING OF EXTENDED DEFECTS IN CRYSTALLINE MATERIALS AND RECENT DEVELOPMENTS OF DESCRIPTION OF ATOMIC INTERACTIONS

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ABSTRACT

Physical and mechanical properties of materials are to a great extent controlled by extended crystal defects: dislocations, interfaces and external surfaces. Very frequently it is the atomic structure and atomic level behavior of these defects which dominate crucial processes. This is the reason why a major effort of atomistic computer simulations in materials science has been modeling of such defects. An essential precursor of all atomistic studies of systems composed of many atoms is a method for evaluation of the energy of such system as a function of positions of all the atoms. For this reason we first summarize such methods ranging from density-functional theory based calculations to pair-potentials and many-body central force interactions. We discuss in more detail the tight-binding approach in the formulation of bond-order potentials. This is a real space treatment suitable for studies of extended defects that is capable to deal physically correctly with the mixed metallic and covalent bonding and is thus applicable to transition metals and their alloys, such as TiAl.

The most significant atomistic calculations have always been those the goal of which was to attain physical understanding of complex atomic level phenomena and their relation to macroscopic properties. Such studies have usually been performed using a relatively simple description of atomic interactions although often linked with more fundamental electronic structure based calculations. Two such studies are presented in this paper. The first deals with segregation of bismuth to grain boundaries in copper and associated embrittlement. Based on the results of atomistic modeling it is argued that embrittlement is associated with formation of certain two-dimensional phases in grain boundaries and that such structures are only formed for particular orientations of the boundary plane after a sufficiently high concentration of bismuth has accumulated. At the same time this may be the reason for segregation induced faceting. This mechanism may not be specific to Cu-Bi but may operate in other systems.

The second example is modeling of 1/2[111] screw dislocations and their motion in bodycentered cubic transition metals, specifically Mo and Ta. We concentrate on the break down of the Schmid law and demonstrate how understanding of this phenomenon, attained on atomic level, can be transferred to the continuum analyses of deformation of these materials.

KEYWORDS

Potentials: pair, many-body, bond-order, TiAl, copper-bismuth, segregation, embrittlement, bcc transition metals, dislocation core, non-Schmid behavior, constitutive equations

INTRODUCTION

Computer simulation is a methodology which allows us to investigate spatial and temporal development of models that represent complex physical systems which cannot be studied by analytical methods. By comparing the simulation results with experiments and approximate theoretical analyses we can test the validity of the models and the underlying theories. This, in turn, leads to further improvement of the models and thus of understanding of properties of the systems studied. However, since the computer simulation often provides much more detailed information on microscopic structures and phenomena than what is accessible experimentally, it may also lead to development of new concepts and predictions of new types of behavior. It is the synergistic relationship between experiments and theory promoted by the computer simulation studies that makes the computer modeling a very valuable tool in many branches of science and engineering. In materials science computer modeling studies presently range from phenomenological modeling of material processing to first-principle quantum mechanical simulations of atomic and electronic structures and atomic level mechanisms [1-3].

Atomic level computer modeling, which is the topic of this paper, has a potential to open new avenues in studies of microscopic origins of material behavior and it has, indeed, become one of the major research tools in materials science [4-8]. In such calculations we are usually investigating structures and structural changes of a system composed of a very large number of particles which interact in a complex non-liner manner. The methods used in these calculations are: (i) Molecular statics, employed in calculations not involving temperature, principally a procedure for finding minima of functions of many variables. (ii) Molecular dynamics in which either classical or quantum mechanical equations of motion are solved by numerical means. (iii) Monte Carlo employing equilibrium classical or quantum statistical mechanics in the formulation of microcanonical, canonical and grand-canonical ensembles. All these methods are fairly standard (see e. g. [9]) although modifications and improvements are being developed continuously in conjunction with simulation studies.

A major effort of atomistic computer simulations in materials science has been modeling of extended crystal defects such as interfaces, external surfaces, dislocations, inclusions and flaws such as cracks. The reason is that physical and mechanical properties of real materials are to a great extent governed by such defects and very frequently it is their atomic structure, atomic level behavior and atomic level processes associated with them that dominate phenomena controlling macroscopic properties of materials. The two well known examples are segregation of alloying elements to interfaces, grain boundaries and surfaces that is confined to a few atomic layers and yet completely changes cohesive and chemical properties of these regions [10-15], and the role of dislocation cores in plastic deformation that dominates, for example in bcc metals [16-20] and intermetallic compounds [21-23], the temperature dependence and crystallography of plastic flow.

In order to carry out atomistic studies of a systems composed of many atoms we need to know how to evaluate the energy of such system as a function of positions of all the atoms. On the most fundamental level this can be done, using the adiabatic approximation of separating atomic nuclei and electrons, by solving the corresponding quantum mechanical problem and evaluating the total energy as a sum of interaction energies of the nuclei and the energy of the electrons. A series of approximate solutions of this problem has been developed ranging from so called ab-initio calculations carried out in the framework of the density functional theory [24-26] to simple empirical schemes (see e. g. [5]). These approaches will be discussed briefly in the following section with emphasis on a recent development of bond-order potentials which capture the most important electronic effects and yet allow for large scale simulations [27-31]. The most significant atomistic simulations have always been those which led to a deeper physical understanding of complex atomic level phenomena in broad classes of materials. Such studies generally require serious simplifications of the representation of atomic interactions and the major art in computer modeling is the choice of a sufficiently simple but not oversimplified description of interactions between atoms [32]. In fact, rather crude approximations have often been utilized in such studies and only at a latter stage more sophisticated approaches were introduced in order to investigate aspects specific to certain materials. Examples are analyses of the radiation damage, which were first pioneering computer simulations employing mainly repulsive pair interactions [33], investigations of structures of point defects [34, 35], establishment of the structural unit model of grain boundaries [36, 37] and establishment of the basic features of the cores of screw dislocations in bcc metals [16, 18, 38, 39], all using relatively simple pair potentials; recently calculations employing many-body central force potentials revealed fundamental features of reconstructions and relaxations at surfaces [40-43].

In this paper we present two studies both of which reveal general aspects relevant to our understanding of the fracture and deformation behavior of materials. The first deals with segregation to grain boundaries in the copper-bismuth system. This study leads to the suggestion that boundary embrittlement may result from formation of two-dimensional interfacial compounds, which is frequently linked with faceting. The second study deals with effects of applied stresses on the glide of screw dislocations in bcc transition metals. It reveals the break down of the Schmid law and suggests how this important aspect of deformation behavior can be incorporated into continuum mechanics studies of crystal plasticity.

DESCRIPTIONS OF ATOMIC INTERACTIONS

In any atomistic modeling we need to know how the total energy of the system studied depends on the positions, \mathbf{R}_{i} , of all N atoms forming the system, i. e. we need the function $\mathbf{E}_{tot} = \mathbf{E}_{tot}(\mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_N)$ In principle, this can be provided by electronic structure calculations based on the density functional theory (DFT) [24-26] which are at present the state of the art [3, 44-49]. In the local density approximation (LDA) this problem reduces to solving the Schrödinger-like equation, called Kohn-Sham equation,

$$-\frac{1}{2}\nabla^{2}\psi_{i}(\mathbf{r}) + V_{eff}(\mathbf{r})\psi_{i}(\mathbf{r}) = \varepsilon_{i}\psi_{i}(\mathbf{r})$$
(1)

for the one electron wave functions $\psi_i(\mathbf{r})$ that determine the electron density

$$\mathbf{n}(\mathbf{r}) = 2\sum_{i} \overline{\psi}_{i}(\mathbf{r})\psi_{i}(\mathbf{r})$$
(2)

where the summation extends over the occupied states; the factor 2 arises due to the spin degeneracy. In equation (1)

$$V_{\text{eff}}(\mathbf{r}) = V_{\text{ext}}(\mathbf{r}) + \int \frac{\mathbf{n}(\mathbf{r'})}{|\mathbf{r} - \mathbf{r'}|} d\mathbf{r'} + \mu_{\text{xc}}(\mathbf{n}(\mathbf{r}))$$
(3)

where V_{ext} is the external potential in which the electrons move, for example the potential arising from atomic nuclei or ions, and $\mu_{xc}(n(\mathbf{r})) = d[n(\mathbf{r})\varepsilon_{xc}(n(\mathbf{r}))] / dn(\mathbf{r})$, where $\varepsilon_{xc}(n(\mathbf{r}))$ is the exchange and correlation energy per electron determined at a point \mathbf{r} by the electron density $n(\mathbf{r})$. Various approximations of $\varepsilon_{xc}(n(\mathbf{r}))$ have been proposed and the judicious

choice of this function is a very important component of any DFT-LDA based method. The total energy of the system is then

$$E_{tot} = 2 \sum_{\substack{i \\ \text{occupied}}} \varepsilon_i - \frac{1}{2} \int \int \frac{n(\mathbf{r})n(\mathbf{r'})}{|\mathbf{r} - \mathbf{r'}|} d\mathbf{r} d\mathbf{r'} + \int n(\mathbf{r})(\varepsilon_{xc}(n(\mathbf{r})) - \mu_{xc}(n(\mathbf{r}))d\mathbf{r} + E_{nn}$$
(4)

where E_{nn} is the Coulomb interaction of the nuclei and/or ions. The important difference between the Schrödinger equation and the Kohn-Sham equation (1) is that V_{eff} is a function of the electron density (eq. 3) that is determined by the solutions of this equation, ψ_i (eq. 2). Thus equation (1) has to be solved self-consistently and a number of schemes treating this problem have been developed in the last fifteen years [3, 45-49]. The common feature of all of them is expansions of functions ψ_i into some known set of functions that form a complete system in terms of the Sturm-Liouville problem. In this representation equation (1) becomes a set of homogeneous linear equations for the expansion coefficients and ε_i are the corresponding eigenvalues. This problem can be treated in real space for finite, generally small, clusters. However, in most cases periodic boundary conditions are employed to mimic an infinite system and the Bloch theorem is utilized. In this case only the atoms within the repeat cell are independent and at present such calculations can be carried out comfortably when the number of these atoms is of the order of hundred.

Such calculations are now used routinely in studies of the relative stability of even rather complex crystal structures (see e. g. [50-52]), when evaluating elastic moduli, and they have also been employed in studies of ideal strength of materials [53-55]. However, DFT-LDA calculations of extended defects are still very limited, usually to those cases for which small periodic repeat cell does not represent a severe limitation. Examples are studies of certain short period grain boundaries (e. g. [56-58]), energy-displacement surfaces (γ -surfaces) for planes with small unit cells (e. g. [59-62]) and studies of cores of straight dislocations with short periods along the dislocation line, for example partial dislocations in silicon (e. g. [63-67]) and screw dislocations in molybdenum and tantalum [68, 69]. However, in the latter case the requirement of three-dimensional periodicity enforces that calculations are made for networks of dipoles rather than for individual dislocations which is a severe limitation, in particular when dislocation motion is to be studied.

However, interesting extended defects are often those with large repeat cells and, furthermore, studies of dislocations and interfaces frequently require extensive relaxations and investigations of many different configurations so that studies based solely on DFT-LDA are not feasible. The prime example is investigation of the motion of dislocations under variously applied stresses that may have to be carried out for hundreds of cases [70-72]. For this reason most atomistic studies of dislocations, interfaces, cracks and other extended defects have been made using relatively simple descriptions of atomic interactions [73]. For metallic materials, pair-potentials were the most common in the early developments (for reviews see [74, 75]) while in recent years the most popular are the central-force many-body potentials in the formulation of the embedded atom method (EAM) [40, 76, 77] and/or Finnis-Sinclair type potentials [78]. These developments are briefly reviewed below. For ionic solids pair-potentials and the shell model have been used most frequently (see e. g. [79, 80]) but these studies are outside the scope of this paper.

Potentials including non-central interactions, applicable to both metals with some covalent bonding (transition metals) and covalently bonded solids, have been developed more recently (see e. g. [81-91]). An important advancement, based on the tight-binding method, is construction of bond-order potentials, originally proposed by Pettifor and co-workers [29-31, 92-95]. These potentials have now been developed for a number of transition elemental metals as well as for some alloys and these recent advancements will be reviewed below.

Pair potentials and many-body central force potentials

Description of atomic interactions by pair potentials was first introduced for inert gasses, where the interactions are of Van der Waals type, and for molecular dimers. The two most famous potentials used in these two cases are the Lennard-Jones [96] and the Morse potential [97], respectively. Potentials of this type have been frequently employed in solids and proved appropriate for many non-metallic materials. Such potentials are assumed to describe fully the cohesion in a given material and belong to the class of *bond-breaking* potentials [98]. However, this approach is questionable in metallic materials in which the character of bonding is entirely different and cohesion is principally provided by the delocalized electrons that are also responsible for electrical and thermal conductivity. Nevertheless, a different class of pair potentials may be employed when studying metals. These are the *constant volume* potentials [98, 99] and the cohesive energy of the metallic system is then

$$E_{coh} = \frac{1}{2} \sum_{i \neq j=1}^{N} V_{ij} (r_{ij}) + U(\rho)$$
(5)

where V_{ij} is the pair potential describing the interaction between the atoms i and j, generally of different type, and U(ρ) is the part of the energy that depends on the average density of electrons, ρ , directly related to the material density. The bulk of the cohesion is included in U(ρ) and the pair potential describes the energy changes associated with the variation of atomic configurations at constant density and/or volume.

Such potentials were derived from first principles for s- and p-bonded metals (alkali metals, aluminum etc.) in the framework of the weak pseudopotentials [100, 101]. An example is the pair potential for aluminum derived by Dagens et al. [102]. In this case the pair potential contribution to the cohesive energy is actually positive, which emphasizes that the cohesion is provided by the density dependent term. At the same time many features of grain boundaries in aluminum were revealed using this potential in constant volume calculations [36, 103-105]. Potentials of this type are generally long-ranged and for large values of r exhibit Friedel oscillations of the type $\cos Qk_F r)/r^3$, where k_F is the Fermi vector; a method for damping these potentials has been proposed in [106]. However, many short-ranged empirical potentials of this type have been proposed [74, 75, 107]. The most famous is the Johnson's potential fitted to equilibrium properties of iron [34, 35]¹.

The dependence of U on the average density of the material is a serious limitation in atomistic studies since significant local changes of the density may occur in the cores of extended defects and this needs to be taken into account. This problem has been to some extent alleviated by introduction of many-body central force potentials, specifically the EAM

$$C_{11} = \frac{1}{2\Omega} \sum_{\substack{i,j \\ i \neq j}} \Psi(r_{ij}) \frac{(r_{ij}^{\alpha=1})^4}{r_{ij}^2} - \frac{dU}{d\Omega} + \Omega \frac{d^2U}{d\Omega^2} \quad C_{44} = \frac{1}{2\Omega} \sum_{\substack{i,j \\ i \neq j}} \Psi(r_{ij}) \frac{(r_{ij}^{\alpha=1})^2 (r_{ij}^{\alpha=2})^2}{r_{ij}^2} - \frac{dU}{d\Omega}$$
$$C_{12} = \frac{1}{2\Omega} \sum_{\substack{i,j \\ i \neq j}} \Psi(r_{ij}) \frac{(r_{ij}^{\alpha=1})^2 (r_{ij}^{\alpha=2})^2}{r_{ij}^2} + \frac{dU}{d\Omega} + \Omega \frac{d^2U}{d\Omega^2} \quad \text{where} \quad \Psi(r_{ij}) = \frac{d^2V_{ij}(r_{ij})}{dr_{ij}^2} - \frac{1}{r_{ij}} \frac{dV_{ij}(r_{ij})}{dr_{ij}}$$

where Ω is the volume of the atomic block considered, e. g. the repeat cell. The Cauchy pressure is then

$$C_{12} - C_{44} = 2\frac{dU}{d\Omega} + \Omega \frac{d^2U}{d\Omega^2}$$

Obviously, in the case of bond-breaking pair potentials, when the cohesive energy is determined solely by the pair potential (U=0), the Cauchy relation $C_{12} = C_{44}$ applies.

¹ It is interesting to note that if the cohesive energy is given by equation (5) then in cubic structures the elastic moduli do not satisfy the Cauchy relations ($C_{12} = C_{44}$), often regarded as an obvious consequence of pairpotentials. In fact, in this case the elastic moduli are given as

[40, 76, 77] and Finnis-Sinclair type potentials [78]. In the framework of these empirical schemes the cohesive energy is again given by equation (5) but

$$U(\rho) = -\sum_{i=1}^{N} F_i(\rho_i)$$
(6)

where F_i is the many-body and/or embedding function associated with the atom i. It is a function of a quantity ρ_i that is either equal or related to the electron density at the site i. The form of the function F_i is chosen on the basis of more fundamental physical considerations. In EAM this is determined using arguments based on the local density functional theory [40, 76]. In the case of Finnis-Sinclair potentials, which are based on the second-moment approximation to the density of states in the tight-binding theory incorporating charge conservation, $F_i = \sqrt{[78, 108]}$. In both schemes

$$\rho_{i} = \sum_{i} \Phi_{ij}(\mathbf{r}_{ij}) \tag{7}$$

where Φ_{ij} are short-ranged pair-potentials, generally dependent on species at sites i and j. The physical interpretations of these potentials somewhat differs in the two schemes. In EAM they are taken as contributions to the density of electrons at the site i arising from neighboring sites j. Thus these functions are fixed in advance of fitting and the embedding function, together with the pair potential V_{ij} , are fitted to reproduce correct equilibrium lattice structure, cohesive energy, elastic moduli and other experimentally determined equilibrium properties and/or other quantities obtain from DFT-LDA calculations. In the Finnis-Sinclair scheme F_i is fixed and potentials Φ_{ij} , interpreted as squares of hopping integrals [108], are fitted together with the pair potential V_{ij} .

Both EAM and Finnis-Sinclair type potentials have been constructed for many elemental metals and binary alloys. In the following section we shall present studies of grain boundaries in the Cu-Bi system. The important aspect of the construction of potentials for this system, performed in [109], was fitting to the equilibrium lattice parameter, the bulk modulus, the tetragonal shear modulus, $\frac{1}{2}(C_{11}-C_{12})$, and the trigonal shear modulus, C_{44} , for the hypothetical compound Cu₃Bi with the L1₀ structure, determined by DFT-LDA based all-electron full-potential linear-muffin-tin-orbital method (FP-LMTO) [110]. In this way the size of the Bi atom embedded in Cu was correctly estimated and the size effect is possibly the governing parameter when studying this alloy.

However, in spite of the large success of EAM and many-body central force potentials generally, these schemes are limited to materials in which the covalent bonds are either non-existent or only weak. Thus the most successful applications were for noble metals and their alloys and Ni-Al alloys (see e. g. [111, 112]) though potentials for bcc transition metals have also been developed and used quite successfully [20, 72, 113]. Yet, as discussed below, analogous schemes for hcp Ti [114] and tetragonal (L1₀) TiAl [115, 116] are more limited. Within the EAM this problem has been tackled by introducing empirically the angular dependence into ρ_i in equation (7) [85, 87, 90, 91]. However, the approach which comprises the covalent character of bonding intrinsically is the tight-binding method which forms the basis of the treatment discussed in the following section.

Tight-binding method and bond-order potentials

The main aspect of the descriptions of interatomic forces which comprise the covalent character of bonding is that the cohesive energy depends not only on the separations of the atoms but also on the angles between pairs of bonds. This is obviously essential in covalently bonded solids, such as silicon, but may also be very important in transition metals and alloys

involving transition elements [117]. The approximate approach which can be employed to treat this problem is the tight binding method with the two-center orthogonal approximation [28, 100, 118]. In this approach the one-electron wave functions are solutions of the equation which looks formally the same as equation (1) but V_{eff} is no more dependent on the electron density but it is a fixed potential. Thus the one electron functions, ψ_i , are solutions of a Schrödinger equation but the main problem is the appropriate choice of the Hamiltonian which contains the potential that is now fixed.

The tight-binding technique then proceeds by expanding the one electron functions ψ_i into atomic-like orbitals centered at individual atoms and the tight-binding Hamiltonian is then

$$\mathbf{H}_{\mathsf{TB}} = \sum_{\mathsf{I},\mathsf{J}} \mathbf{H}_{\mathsf{I},\mathsf{J}} |\mathsf{I}\rangle \langle \mathsf{J}$$
 (8)

Here index $I \equiv [i, L_i, s_i]$, where i numbers the atomic sites, $L_i = (\ell, m)_i$, where ℓ denotes the quantum orbital moment and m the quantum magnetic moment for spherical symmetry, and s_i marks the type of species at the sites i; analogously $J \equiv [j, L_j, s_j]$, $L_j = (\ell, m)_j$. $||\rangle$ then represents an atomic-like orbital of symmetry determined by L_i at the site i; $\langle J \rangle$ has analogous meaning. The summations in equation (8) extend over all atomic sites and orbitals, respectively. In the two-center approximation the angular dependence of the Hamiltonian elements $H_{i,J}$ is thus detached from their dependence on separation of atoms i and j, r_{ij} , and for atomic type orbitals of s, p, d and f types this dependence has been determined by Slater and Koster [119]. Hence, in any tight-binding scheme one needs to establish the dependence of $H_{i,J}$ on r_{ij} for $i \neq j$ and the values of the on-site elements for i = j. In earlier studies these Hamiltonian elements were usually determined by fitting to experimental data [100] and more recently they are being ascertained on the basis of DFT-LDA calculations.

In the standard tight-binding scheme the cohesive energy is divided into the band energy, arising from formation of the valence band, and the part described by a repulsive pair potentials [100]. However, it has been shown [27, 120, 121] that by subtracting the on-site Hamiltonian elements from the band energy a more appropriate division of the cohesive energy is obtained. This division into the bond energy, U_{bond} , and another part which can still be represented by a pair-potential, is central for the development of bond-order potentials (BOP). Within this scheme

$$U_{\text{bond}} = \sum_{\substack{I, J \\ i \neq j}} H_{I, J} \Theta_{J, I}$$
(9)

where Θ_{JI} are bond order matrix elements. Thus the bond energy associated with atom i, is within the BOP method decomposed explicitly in terms of the contribution from individual bonds which atom i makes with the neighboring atoms j [28]. The bond-order matrix can be expressed for a given Hamiltonian in terms of the derivative of certain diagonal elements of the Green's function [94, 122]. These diagonal elements are evaluated using the recursion method of continued fractions [123] with the recursion coefficients determined by the Lanczos algorithm [124]. When evaluating the bond-order matrix the on-site Hamiltonian elements are also needed. These are adjusted self-consistently to maintain local charge neutrality with respect to each atom. This condition reflects the perfect screening properties of metallic materials [28]. The relatively complex procedures involved in evaluation of U_{bond} , including the attainment of charge neutrality, are all part of the suit of computer codes available as the Order N (OXON) package and are described in more detail in [30, 125, 126]. Within this scheme forces on atoms are calculated directly employing the Hellman-Feynman theorem [127, 128] for the bond part of the energy. Recently, it has been found that it is not possible to reproduce with sufficient precision the Cauchy pressures if U_{bond} is supplemented only by a pair potential interaction. In fact, negative Cauchy pressures, encountered in compounds such as TiAl, could not be reproduced at all [129]. For this reason, in the latest version of BOP the cohesive energy is written as

$$\mathsf{E}_{\mathsf{coh}} = \mathsf{U}_{\mathsf{pair}} + \mathsf{U}_{\mathsf{bond}} + \mathsf{U}_{\mathsf{env}} \tag{10}$$

where U_{pair} is the repulsive interaction between the atoms described by a pair potential and

 U_{env} is the environmentally dependent part of the energy which represents the s, p ion core repulsion and it is described by a repulsive central-force many-body potential which was proposed to have the screened Yukawa form [129]. This functional form is described in more detail in [130, 131].

The construction of BOPs then proceeds by sequential fitting. This means that first U_{bond} is constructed based solely on data obtained from DFT-LDA calculations with no empirical input. At this stage the numbers of electrons of s, p, d etc. symmetries have to be chosen so as not to be far from the values found in DFT-LDA calculations and the number of levels included in the Lanczos algorithm must be selected so as to achieve sufficient precision. Next U_{env} is obtained by fitting the Cauchy pressures and, finally, the pair potential is fitted so as to reproduce several equilibrium properties, namely, lattice parameters, remaining elastic moduli and cohesive energy. The BOPs have recently been developed for several transition metals with the bcc structure [132, 133], titanium [126, 131] and Ti-Al alloys [130, 131]. For the elemental metals only d electrons were included into the calculation of U_{bond} while in Ti-Al dorbitals centered on Ti and p-orbitals centered on Al were included. The functional form of the dependence of the Hamiltonian elements, called bond-integrals, on the separation of atoms (i. e. scaling) was determined by calculations employing the first-principles TB-LMTO [134]. In this method the Hamiltonian has a simple analytical form that relates to a two-center, orthogonal tight-binding Hamiltonian so that a direct link with the tight-binding method can be established. This form was then approximated analytically by an inverse power law or by the functional form suggested by Goodwin, Skinner and Pettifor [135]. Recently. environmental screening of bond integrals has been introduced [136]; this is most important for Mo and Mo-Si alloys. In the following we present several examples which demonstrate the superiority of BOP over central forces because directional bonding is correctly taken into account

The first is the study of dislocations in titanium the purpose of which was to explain the preference for prismatic slip in this metal [137]. Both the BOP [126] and a central-force Finnis-Sinclair type potential for Ti [114] has been used to study atomistically the core structure of the $1/3 < \overline{1210} >$ screw dislocation. This dislocation may either dissociate into Shockley partials on the basal plane or spread in a continuous manner into the prism plane where no well-defined stacking fault exists. The spreading of the dislocation core into the prism plane is always energetically favored over the splitting into the basal plane in the case of BOP whilst the opposite has been found in the case of the central-force Finnis-Sinclair type potential. 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 BOP that splitting into Shockley partials is not energetically favorable. The reason for such a high stacking fault energy is the non-central character of atomic interactions in titanium arising due to the significant contribution of d-electrons to the bonding, which is correctly captured by the bond-order potential. Hence, the results obtained using the BOP explain the strong preference for the prism slip over the basal slip in titanium.

The second example is the study of highly distorted structures of Mo and Ta encountered along a certain deformation path. The most common path of this type is the Bain deformation path between the bcc and fcc lattices [138] but other more complex paths were defined

recently [139]. Here we show the study of the trigonal path which is also a deformation path between the bcc and fcc lattices but passing through the simple cubic (sc) structure. Starting from the bcc lattice, the trigonal path follows the homogeneous deformation corresponding to the extension along the [111] axis while keeping the atomic volume constant. In the coordinate system with the x, y and z axes parallel to $[1\overline{10}]$, $[11\overline{2}]$ and [111] directions it is described by the Lagrange strain tensor for large deformations

$$\varepsilon_{11} = \varepsilon_{22} = (p^{-2/3} - 1)/2 \quad \varepsilon_{33} = (p^{4/3} - 1)/2 \quad \varepsilon_{12} = \varepsilon_{13} = \varepsilon_{23} = 0, \quad (11)$$

where p is a parameter characterizing the deformation; it varies from 1 for bcc, through 2 for sc to 4 for fcc lattices [139]. The magnitude of the vectors parallel to the first two directions is proportional to $p^{-1/3}$ while the magnitude of the vectors parallel to the [111] direction is proportional to $p^{2/3}$.



Fig. 1. Comparison of calculations of the energy per atom of the structure deformed along the trigonal path using BOP, DFT-LDA and FS potential, respectively. (a) Molybdenum; (b) Tantalum.

The dependence of the energy per atom for Mo and Ta, relative to the energy for the bcc lattice, on the parameter p is shown in Figs. 1a, b. Calculations employing the BOP are compared in these figures with calculations made within DFT-LDA using FLAPW code [140, 141] and also Finnis-Sinclair (FS) type central-force many-body potential [113]. The extrema for p = 1, 2 and 4, corresponding to different cubic structures, are dictated by the symmetry. However, auxiliary minima found in the vicinity of p = 4 for Mo are specific to this material; they were also found for Nb [132] but not for Ta, as seen in Fig. 1b. Both situations are well reproduced by BOP but not by the central-force potentials. The latter lead to a local minimum for the fcc structure in both Mo and Ta while DFT-LDA and BOP suggest that in Mo the fcc structure corresponds to a local maximum with subsidiary minima on each side of this maximum. Clearly, this feature is rather subtle since only small energy differences are involved and demonstrates that BOP is capable to capture such features even though the corresponding structures are very far from the equilibrium bcc lattice for which the fitting has been made. In other parts of the calculated energy vs p dependence the agreement between BOP and DFT-LDA calculations is very good while more significant deviations are seen for the FS potentials.

The third example shows results of calculations of energies of fully relaxed structures of antiphase domain boundary (APB), complex stacking fault (CSF) and superlattice intrinsic stacking fault in TiAl with tetragonal $L1_0$ structure. The results obtained using the recently constructed BOP for TiAl [131] are compared in Table 1 with DFT-LDA calculations employing FP-LAPW [140, 141] and FT-LMTO methods, calculations using Finnis-Sinclair type potential [115], as well as available experimental measurements. Obviously, the BOP results are in the same range as results obtained in DFT-LDA calculations. Importantly, the

relatively high energy of the SISF is correctly reproduced by BOP. In this fault the separations of the first and second nearest neighbors are practically the same as in the ideal $L1_0$ lattice and in the framework of central forces the only contributions to the fault energy arise from more distant neighbors. For this reason FS potentials lead to a very low energy of the SISF. This suggests that the relatively large energy of the SISF results from changes in bond angles and the BOP scheme captures this effect accurately. While the calculated energy of the SISF also agrees very well with the measurements the calculated energies of the APB are generally higher. However, the measurements may be affected by a strong dependence of this energy on composition [142] while calculations were all made for the stoichiometric composition.

Furthermore, it is remarkable that the BOP for Ti-Al alloys also predicts correctly that the hexagonal DO_{19} structure is the most stable structure for the 3:1 composition although no properties of Ti₃Al were used when fitting the potentials. For this composition the competing structure is the cubic L1₂ and its energy was found to be by 17.3 meV/atom higher than that of the DO₁₉ structure; the FP-LMTO calculations show the preference by 9.5 meV/atom (D. Nguyen-Manh, private communication). Moreover, the BOP predicts very closely the correct lattice parameters and cohesive energy of the DO₁₉ Ti₃Al.

Table 1. Energies of APB, CSF and SISF in TiAl in mJ/m² calculated using four different methods together with experimentally measured values: (a) [143], (b) [144], (c) [145], (d) [146]. In (a), (b) and (d) the alloy composition was $Ti_{46}Al_{54}$ and in (c) $Ti_{44}Al_{56}$.

	BOP	FP-	FP-	FS	Experiments			
		LAPW	LMTO		(a)	(b)	(c)	(d)
APB	545	667	710	275	250	190	198	>250
CSF	412	362	314	275				
SISF	140	172	134	2.9	140	105	116	140

EXAMPLES OF ATOMISTIC STUDIES RELEVANT TO FRACTURE AND PLASTIC DEFORMATION

Grain boundaries in copper-bismuth alloys

Copper-bismuth alloy is a very suitable model material for investigation of the segregation and embrittlement phenomena. The solubility of Bi in Cu is very low [147] and segregation to grain boundaries and associated embrittlement has been observed in this system long time ago [148-151]. A remarkable phenomenon observed in this system is the segregation induced faceting [152-159] which occurs after a saturation level of bismuth in grain boundaries has been reached. This process is reversible and de-faceting occurs as bismuth dissolves during annealing at a higher temperature [155]. Recently several experimental studies of segregation and faceting have been made and linked with computer simulations which were carried out using the central-force Finnis-Sinclair type potentials for Cu-Bi system, constructed in [109] and briefly described in the section on potentials.

Using high-resolution Z-contrast imaging the positions of Cu columns and Bi-rich atomic columns in the Σ =5(310) symmetrical tilt boundary were unambiguously identified in Ref. [158, 159]. These observations agree very closely with the results of atomistic modeling of this boundary [160] which are shown in Fig. 2. This structure was found by molecular statics calculation in which the replacement of Cu by Bi was tested at various sites within the repeat cell of the boundary. Recently, we carried out a study of the segregation to this boundary using the modified canonical ensemble Monte Carlo developed in [161]. Fig. 3

shows a typical cross section through this boundary after a large number of Monte Carlo steps at the temperature of 300 K. It is seen that this structure is very close to that shown in Fig. 2 and thus also to that observed experimentally [158, 159]. The most remarkable finding is that a well-defined two-dimensional Cu-Bi structure is formed in this boundary as a result of segregation. As will be discussed below, this may be a general phenomenon.



Fig. 2. Structure of the Σ =5(310) symmetrical tilt boundary containing Bi, shown in the projection of the tilt axis ([001]), calculated by a molecular statics method. Small gray circles represent columns of Cu atoms and large dark circles columns of Bi atoms.



Fig. 3. One lattice spacing thick cross section of the Σ =5(310) symmetrical tilt boundary containing Bi, shown in the projection of the tilt axis ([001]), calculated by the modified canonical ensemble Monte Carlo method for the temperature of 300K. Small gray circles represent Cu atoms and large dark circles Bi atoms.

The segregation of Bi is in general rather different to different boundaries, as demonstrated, for example, in the recent study of segregation in bicrystals with boundaries of different albeit well defined misorientations and boundary plane orientations [158]. One of the most interesting situations arises in the case of Σ =3 boundaries (tilt axis of the <110> type). No segregation occurs at such boundaries when the boundary plane is of the {111} type, i. e. at coherent twins [158, 162, 163]. On the other hand, incoherent, generally curved Σ =3 boundaries were observed to facet in Cu-Bi such that at least one of the facets was the coherent twin [156, 157, 164]. While a similar faceting may occur even in pure copper [165], the {111} facets in Cu-Bi formed when the corresponding incoherent boundaries contained certain amount of Bi.

An analysis employing high resolution electron microscopy (HREM) suggests that these {111} facets contain a high concentration of bismuth and their structure can be described as follows [109, 166, 167]. In the framework of the 'ABC' stacking of {111} atomic planes in an fcc crystal, the $\Sigma=3$ (111)/(111) twin in pure copper can be represented as

where the vertical lines mark the position of the boundary. The structure with Bi could be represented in the same way but in the layer C at the boundary one third of the copper atoms are replaced by hexagonally arranged Bi atoms. However, the Bi atoms are centered outside this atomic plane so that a physically appropriate representation of the model structure is

where C' denotes a plane of copper atoms in which one third of the atoms were replaced by hexagonally arranged vacancies, and C(Bi) the plane of bismuth atoms positioned above these vacancies. In order to investigate the feasibility of this structure atomistic calculations were carried out using the same many-body central-force potentials as in the study of the $\Sigma=5(310)$ boundary [109, 167]. The calculated fully relaxed structure is shown in Fig. 4a in the projection along the tilt axis [110] and in Fig. 4b in the [111] projection showing the planes C' and C(Bi).



Fig. 4. Structure of the $\Sigma = 3$ (111)/(111) tilt boundary containing Bi. (a) Projection along the tilt axis [110]. (b) [111] projection showing the planes C' and C(Bi). Small gray circles represent Cu atoms and large dark circles Bi atoms.

In order to make a detailed comparison of the calculated and observed structures, a series of images, corresponding to the same defocus conditions and thickness as in the HREM study, were calculated for the relaxed structure using the multislice formalism [168]. There is an almost perfect match between the calculated and observed image and even quantitative features such as total expansion, i.e. the relative displacement of the two grains in the direction perpendicular to the boundary, are within the experimental limits of the accuracy [109].

In order to assess whether this structure is not related to some possible three-dimensional phases which could then grow into the bulk, DFT-LDA based calculations of possible related structures have been made using the full-potential LMTO method [169, 170]. These calculations demonstrate that the structure found is purely a grain boundary phase. Recently, we have used the modified canonical ensemble Monte Carlo method to investigate the stability of this structure and these calculations show that it is stable with respect to the dissolution of bismuth at temperatures well above the room temperature.

These combined experimental and computer modeling studies suggest that the $(111)/(11\overline{1})$ facets, formed from general curved boundaries when a sufficient amount of Bi segregated to them, contain a two-dimensional ordered Cu-Bi phase. However, the same structure cannot be formed by direct segregation to the coherent twin. This phenomenon may be more general. Recently Sigle et al. [171] studied segregation in the bicrystal of a Cu-Bi alloy containing

originally the symmetrical tilt $\Sigma 19$ {331} boundary. This boundary was found to facet into two asymmetrical tilt boundaries with the boundary planes {211}/{210} and {332}/{110}, respectively. The concentration of Bi at the facets was found to be significantly higher than in the non-faceted region of the boundary. Furthermore, fracture occurred readily at faceted boundaries while non-faceted parts of the boundary did not appear embrittled although they did contain a significant amount of segregated bismuth. Such high propensity of cracking along boundary facets formed as a result of Bi segregation has already been observed by Donald and Brown [153]. While detailed atomic structure of the $\Sigma 19$ facets could not be determined in [171], it is possible than an ordered two-dimensional phase has formed in these facets, similarly as in the $\Sigma = 3$ (111)/(111) facets.

These studies suggest that embrittlement invoked by segregation of bismuth to grain boundaries in copper is associated with formation of certain two-dimensional phases in these boundaries. In some of them, for example in the Σ =5(310) symmetrical tilt boundary, such an ordered structure is formed directly as the result of segregation. This boundary has, indeed, been found to be embrittled [158]. In other boundaries such structures are only formed for certain orientations of the boundary plane and only after a sufficiently high concentration of bismuth, which is originally randomly distributed, has accumulated by segregation. This aggregation of bismuth may then be the driving force for faceting which has been frequently observed. We conjecture that this is the case in Σ =3 and Σ 19 boundaries. The embrittlement is then not simply related to the decrease of cohesion due to the presence of bismuth but a result of formation of an ordered phase which may not only decrease cohesion but also hinder the dislocation activity in the vicinity of the boundary. This mechanism of embrittlement may operate in other systems than Cu-Bi. For example faceting of similar type was also observed in iron doped with tellurium after tellurium segregated to grain boundaries [172].

Dislocations in bcc metals and break down of the Schmid law

Some of the early atomistic studies of dislocations were done for bcc metals since their plastic behavior is strikingly different than that of fcc metals (for reviews see [17, 18, 173-175]). In the latter case the slip systems are always $<110>{111}$, the critical resolved shear stress (CRSS) is small (of order 10^{-5} G at 4.2 K) and essentially independent of temperature and orientation of loading and it obeys the Schmid law². In the former case the slip directions are the close-packed directions <111> but the slip surfaces, not always planar, may vary with the orientation and sense of the applied stress. The CRSS is high (of order 10^{-2} G at 4.2K) and strongly dependent on temperature and orientation of the applied loads. For example, the CRSS is often very different for loading in tension and compression, respectively. This behavior obviously implies that the Schmid law is not valid. In fact there is no crystallographic reason why shearing in opposite directions along <111> should be equivalent since the {111} plane is not a mirror plane in bcc lattice; this is in contrast with the {110} plane which is perpendicular to the <110> slip direction in fcc crystals and guaranties the equivalence of the two senses of slip.

Many experimental and theoretical studies performed in the last forty years have unequivocally established that the core structure of 1/2 < 111 screw dislocations controls

 $^{^2}$ It is not always recognized that the Schmid law contains two distinct assertions. The first, more widely known, that glide on a given slip system, defined by a slip plane and direction of slip, commences when the resolved shear stress on that system, the Schmid stress, reaches a critical value [176]. The second part of the Schmid law implicitly assumes that this critical stress is not influenced by any other component of the applied stress tensor. Thus the stress tensor components regarded as insignificant are: (i) Shear stresses in the direction of slip acting in crystallographic planes other than the slip plane. (ii) Stress tensor components that cannot drive the glide in the slip direction, for example shear stresses in the direction perpendicular to the direction of slip.

these aspects of the plastic behavior of bcc metals. A number of comprehensive reviews that deal with this topic are available [16-18, 173-175, 177]. The most prominent characteristic of the core of 1/2 < 111 screw dislocations is its possible spreading into several non-parallel planes of the <111 zone. This possibility was first recognized by Hirsch [178] and it became the guiding idea of studies of the plastic behavior of bcc metals.

Already the early atomistic calculations, carried out using pair potentials, demonstrated this fundamental feature of the screw dislocation cores in bcc metals [16, 38, 39, 179]. Furthermore, they revealed a complex response of these dislocations to applied stresses [70, 180, 181], in particular the well-known twinning-antitwinning asymmetry of shear in {112} planes. While some of these aspects of plastic behavior are common to all metals with bcc structure, large quantitative differences arise in the magnitudes of asymmetries of slip geometry and flow stress and qualitative differences occur in the tension-compression asymmetry which cannot be fully related to the asymmetry in the sense of shearing. Owing to the renewed interest in understanding plastic behavior of transition bcc metals, the structure and properties of screw dislocations were investigated using a variety of methods, ranging from DFT-LDA calculations [68, 69], through potentials based on generalized pseudopotential theory [82, 83] that include non-central interaction [182-184], to central-force many-body potentials [20, 72] constructed in [113]. In [72] the response of dislocations to applied loads was studied in detail and thus non-Schmid effects in the plastic yielding of these materials investigated. We present here some of the important findings of this study and discuss how these can be linked with macroscopic continuum modeling of plasticity in these metals.



Fig. 5. Displacement maps of the cores of screw dislocations in Mo (a) and Ta (b). (c) Orientations of all the $\{110\}$ and $\{112\}$ planes belonging to the [111] zone.

The calculated core structures of screw dislocations in tantalum and molybdenum are shown in Figs, 5a and b using the method of differential displacements for the screw component of the displacements³. To facilitate understanding of these pictures the orientations of all the $\{110\}$ and $\{112\}$ planes belonging to the [111] zone are shown in Fig. 5c. In the case of molybdenum the core is relatively widely spread into three $\{110\}$ planes of the [111] zone. Since the core structure shown in Fig. 5a is not invariant with respect to the [101] diad, a symmetry operation of the bcc lattice, another energetically equivalent configuration, related by this symmetry operation, must exist. Hence, the dislocation core may exist in two symmetry related variants and, therefore, this core configuration is called degenerate.

³ The atomic arrangement is shown in the projection perpendicular to the direction of the dislocation line ([111]). The circles represent atoms within one period without distinguishing that they are positioned in three different layers separated by the distance $a\sqrt{3}/2$. The pictures are all oriented such that the horizontal rows of atoms correspond to (101) planes. The chosen component of the relative displacement of the neighboring atoms produced by the dislocation is depicted as an arrow between them. The length of the arrows is proportional to the magnitude of the displacement normalized by |a/d[111]|; the direction of the arrows represents the sign of the displacement.

Furthermore, the displacements inside the core also possess significant edge components perpendicular to the total Burgers vector. This type of core was recently confirmed in the high-resolution electron microscope study in which the edge components were identified [185]. In contrast, in tantalum (Fig. 5b) the core structure is invariant with respect to all the symmetry operations of the lattice and thus this core structure is called non-degenerate. This core spreads symmetrically into the three {110} planes of the [111] zone, is narrower than in the case of molybdenum, and the edge components are much smaller.

Stressing corresponding to the pure shear in the direction of the Burgers vector can be uniquely represented by the angle χ between the ($\overline{1}01$) plane and the maximum resolved shear stress plane (MRSSP). For such loading the dislocation was found to move in molybdenum along the ($\overline{1}01$) plane for all angles χ but in tantalum along the ($\overline{1}12$) plane. The calculated dependence of the CRSS on the angle χ is shown in Fig. 6 for both molybdenum and tantalum. These results clearly demonstrate that the Schmid law, also drawn in Fig. 6, does not apply. In Ref. [72] the dependence of the CRSS on other stress components was also investigated and this study shows that CRSS also depends on shear stresses perpendicular to the Burgers vector acting in {110} planes. This finding then explains the differences between tension and compression that cannot be associated with the change in the sense of shearing in the direction of the Burgers vector.





Fig. 7. Core structure of the 1/2[111] screw dislocation under the effect of applied stresses. (a) and (b) Mo and Ta, respectively, with the loading in pure shear in the Burgers vector direction along the $(\overline{1} \ \overline{1} 2)$ plane ($\chi = -30^{\circ}$); (c) Mo when the loading is in pure shear in the direction perpendicular to the Burgers vector acting in ($\overline{1}10$) and ($0\overline{1}1$) planes.

The reason for the dependence of the CRSS on other stress components than the Schmid stress is that various shear stress components (which we term non-glide components) alter the cores of 1/2 < 111 screw dislocations prior to the dislocation motion. Examples of such effects are shown in Figs. 7a and b which show the core structures of the 1/2[111] screw dislocations in Mo and Ta, respectively, when the loading is in pure shear in the Burgers

vector direction along the $(\overline{1}\ \overline{1}2)$ plane ($\chi = -30^{\circ}$), at a stress level just below the CRSS. It is seen that in Mo the core extends further into the ($\overline{1}01$) plane while the branches in the other two {110} planes shrink while in Ta the core extends into the ($\overline{1}\ \overline{1}2$) plane. As mentioned above, the glide is on ($\overline{1}01$) planes in Mo and ($\overline{1}\ \overline{1}2$) planes in Ta.

Fig. 7c shows the core of the 1/2[111] screw dislocations in Mo when the loading is in pure shear in the direction perpendicular to the Burgers vector acting in ($\overline{1}10$) and (011) planes. While this non-glide stress does not exert the Peach-Koehler force on the screw dislocation and cannot invoke its motion, it affects strongly the core configuration. When combined with the shear stress acting in the direction of the Burgers vector, which pushes the dislocation along the ($\overline{1}01$) plane, it will hinder the glide and a higher CRSS than without the non-glide stress will result since the core is more widely spread into the ($0\overline{1}1$) plane. On the other hand, when combined with the shear stress acting in the direction along the ($0\overline{1}1$) plane, the corresponding CRSS will be decreased.

Results of the type shown in Fig. 6 can be used to develop constitutive equations for continuum mechanics-based finite element simulations (i. e., yield functions and flow rules) which incorporate the effect of non-glide stresses. This was demonstrated by Qin and Bassani [186, 187] in a continuum model for single crystals. They proposed that a slip system α is at yield when: $\tau^{*\alpha} \equiv \tau^{\alpha} + a_{1}^{\alpha}\tau_{1}^{\alpha} + a_{2}^{\alpha}\tau_{2}^{\alpha} + ... = \tau_{cr}^{\alpha}$, where τ^{α} is the Schmid stress and τ_{k}^{α} (k=1,2, 3..) are the crystallographic non-glide stress components associated with each slip system α ; a_{k}^{α} are the material parameters that determine the relative importance of the different non-glide stresses, and τ_{cr}^{α} is measure of hardness for that slip system. Based upon the results summarized in Fig. 6a it was determined that in the case of Mo the important stress components are shear stresses on (101) and (011) planes [188]. The yield criterion can then be written as

$$\tau^* = \tau_{(101)} + a\tau_{(011)} = \tau_{cr} \quad \Rightarrow \quad CRSS = \tau_{cr} / [cos\chi + acos(\chi + 60)]$$
(12)

The two parameters, a and τ_{cr} , in this yield criterion were determined from a least-square fit of the data in Fig. 6a; $\tau_{cr}/C_{44}=0.0586$ and a=0.641. With these values the CRSS vs χ calculated using the above equation is also plotted in Fig. 6a as a continuous curve. There is excellent agreement with the atomistic simulations and the yield criterion given by equation (12) will then incorporate the core effects found on the atomic level into the continuum analyses of plastic yielding. For a more general state of stress other non-glide stress components will enter the yield criterion.

CONCLUSIONS

Atomic level modeling has become one of the major, rapidly growing areas of materials research. The basic motive follows from the nature of this scientific endeavor. The goal of materials science is to establish relationships between internal structures, ranging from atomic to macroscopic, and properties of materials. This implies that structural features investigated are generally so complex that analytical treatments that have to employ extensive simplifications, may loose the essence of the problem studied. Examples, discussed in this paper, are extended crystal defects that play a major role in the control of mechanical properties of materials. While atomistic modeling in materials research started already in early sixties (e. g. [33, 189]) and played an important role in studies of point defects [34, 35], dislocations and interfaces (for a review see [73]), it became as common as, for example,

microscopy, mechanical testing, electrical and magnetic measurements only in the last ten years. The reason is two-fold. First the immense increase of the computing power allows study of more and more complex and extensive problems. Secondly, and perhaps even more importantly, there has been a very significant advancement in the description of atomic interaction, the most important being the advancement of DFT-LDA based calculations that enable further development of more approximate techniques by providing physical guidelines and inputs.

In this paper we have summarized several of such approximate approaches. The most successful and widely used in the last fifteen years have been the central-force many-body potentials of the EAM [40, 76, 77] and Finnis-Sinclair type [78]. However, as the studies move from relatively simple materials, such as close packed metals and metallic alloys, to materials that are more complex both crystallographically and electronically, the central-force In these materials, such as transition metals, transition metal model is not sufficient. aluminides and silicides, the bonding is frequently mixed metallic and covalent and it is the latter component which has to be properly considered. The DFT-LDA based methods are, of course, fully capable to deal with this problem but their application is still very limited by the size of the atomic block that can be reasonably treated. Very promising approximate approach based on the tight-binding method in the bond formulation [27, 28] is development of bond-order potentials discussed in this paper. It has been shown here that these potentials are, indeed, capable to capture very important aspects of bonding in transition bcc metals and Ti-Al alloys. Furthermore, they have been also very successful in covalent systems, such as silicon and carbon [190-193], and it is expected that they will be similarly profitable in complex systems with mixed covalent and metallic bonding, such as transition metal silicides.

The most consequential atomistic studies have always been those which could attain a general physical understanding of complex atomic level phenomena and their relation to macroscopic properties. Such studies have often been made using a relatively simple description of atomic interactions. The investigation of the segregation of bismuth to grain boundaries in copper and the simulation of the motion of screw dislocations in bcc transition metals are two studies of this type. Both were performed using central-force many-body potentials and thus their validity is limited if directional bonding is of principal significance. Nevertheless, both these studies bring out points that have general significance and applicability.

In the case of grain boundary segregation these calculations suggest that certain twodimensional phases are formed in the boundaries at a certain level of segregation. This may in some cases invoke faceting since such structures are only formed for certain orientations of the boundary plane. The embrittlement may then be the result of formation of such ordered phases which may not only decrease cohesion but also hamper the plastic deformation in the vicinity of the boundary. However, more thorough justification of this notable conjecture, which may have more general implication for understanding of interfacial embrittlement, requires more detailed studies employing methods treating more appropriately the local electronic structures at the boundaries with segregated bismuth and possible two-dimensional ordered phases.

Studies of the motion of screw dislocations in molybdenum and tantalum unveiled which stress tensor components other than the Schmid stress affect significantly the dislocation motion [20, 71, 72]. This allows us to formulate constitutive equations for continuum mechanics-based simulations that account for non-Schmid effects in the plastic behavior of these metals. At the same time this study revealed that two distinct types of screw dislocation core structures, leading to distinct deformation behavior, can exist. They are typified by the core structures found for molybdenum and tantalum, respectively. However, while it is very likely that this finding identified two distinct possibilities that can be

encountered in bcc metals, whether these can be unequivocally associated with molybdenum and tantalum, respectively, again requires calculations employing methods which treat more appropriately the electronic structures and can thus capture irrefutably the differences in bonding between these two transition metals.

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