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# Atomistic modeling of dislocation-interface interactions

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## ABSTRACT

Using atomic scale models and interface defect theory, we first classify interface structures into a few types with respect to geometrical factors, then study the interfacial shear response and further simulate the dislocation-interface interactions using molecular dynamics. The results show that the atomic scale structural characteristics of both heterophases and homophases interfaces play a crucial role in (i) their mechanical responses and (ii) the ability of incoming lattice dislocations to transmit across them.

**Key Words:** interfaces; dislocations; interface shear; molecular dynamics

## 1. INTRODUCTION

Grain boundaries and interphase interfaces in metals have been shown to play a fundamental role in material properties such as strength, fracture, work hardening, and damage evolution under irradiation and shock [1]. Overall, the role of interfaces in plastic deformation of metals encompasses interfaces acting as: (i) sources of defects, (ii) sinks of defects via absorption and annihilation, (iii) barriers to defects, and (iv) storage sites for defects. Previous studies in the literature have often treated the role of interfaces in a phenomenological way, yielding scaling laws such as Hall-Petch that relate strength to the spacing between interfaces that act as barriers to glide dislocations. However, the role that atomic interface structure plays in these responses remains poorly understood and essentially un-quantified.

For coherent interfaces and semi-coherent interfaces that are less complicated than interfaces between non-isostructural phases, coherency stresses play a crucial role in defining the maximum strength that can be achieved. For coherent interfaces in heterophases, the strength model [2] is based on the simple idea that a dislocation cannot traverse the composite unless the net forces on the dislocation in all layers are the same sign. Thus, a stress must be applied that at least cancels the coherency stress in one of the two constituents. For coherent interfaces in single-phase metals, the presence of twin boundaries causes the change of crystal orientations across the

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interface, resulting in the discontinuity of slip systems across twin boundaries, thereby strengthening materials. For semi-coherent interfaces with small misfit (< ≈5%), misfit dislocations relax only the long-range coherency stresses and the interface between the misfit dislocations remains coherent and, therefore, a glide dislocation that intersects the coherent segment of interface in this region still encounters very large stresses.

For interfaces between non-isostructural phases (such as between an fcc and bcc metal) with large misfit (> ≈5%), there are no coherency stresses. Atomic relaxations in the interface are complicated. In this paper, we classify interface structures (with a focus on fcc-bcc systems such as Cu-Nb) into a few types with respect to geometrical factors. Corresponding to these interface types, we study the shear response of interfaces and the dislocation-interface interactions.

## 2. GEOMETRIC-BASED CLASSIFICATION SCHEME FOR THE DEFECT STRUCTURES OF INTERFACES

The atomic structure of interfaces defines their properties and thereby the properties that they impart to polycrystalline and polyphasic materials. Atomic environments inside and in the vicinity of an interface may be distinctly different from those in the neighboring perfect crystals. For interfaces, five variables are needed (Fig. 1) and correspond to the so-called macroscopic degrees-of-freedom, the three that define the orientation relation between the two crystals, and two that define the orientation of the normal to a flat interface. Most other interfaces possess atomic structures may require many variables (microscopic degrees-of-freedom) to adequately define the atomic configuration in and near the interface [3].

Geometric characters of habit planes mainly determine the characteristic of interface structures. From the viewpoint of thermodynamics, interfaces composed of low energy surfaces and/or low energy ledges are energetically favorable, close to thermodynamic equilibrium. Therefore, two geometric factors are chosen to classify interfaces: compact plane and compact direction (Fig. 2a). Besides the two factors, the third factor is the similarity of unit cell because it is likely to form a coherent structure for two habit planes when their unit cells have similar atomic structures (Fig. 2b). With respect to the three geometric factors we classify the experimentally observed Cu/Nb incoherent interfaces with two different orientation relationships (Kurdjumov-Sachs (KS) and Nishiyama-Wassermann (NW)) into five types (Table 1). Using atomistic simulations we studied the characteristics of the five types of interfaces. Fig. 3 shows the atomic structures of a type-4 interface before and after relaxation. Interface defects can be well defined in the relaxed structure coupling with interface defect theory. It is found that the interface plane is flat and contains an array of interface dislocations, dislocations of one set have Burgers vectors that lie within the interface plane due to the lattice mismatch and dislocations of the other set have Burgers vectors normal to the interface due to the non-compact plane in Cu. Comparing the results among the five types of interfaces, we can conclude that (1) the interface plane is flat when one or two of the two habit planes is a compact plane. For example, type 1 interfaces are flat without interface disconnections due to the both compact habit planes as experimentally observed in Cu/Nb films (Fig. 4a) [1, 3, 4]; types 3 and 4 interfaces are flat but contain an array

of interface disconnections due to one compact plane. (2) The interface contains an array of interface disconnections when the compact directions in both crystals are parallel, such as type 2 and type 4. (3) The interface plane becomes faceted when the compact directions in both crystals are parallel. (4) The interface plane is flat and composed of coherent and incoherent regions when atomic structures of unit cell in both crystals are similar (for instance, type 3). However, (5) interface structures become fully disordered when the three conditions are not satisfied.

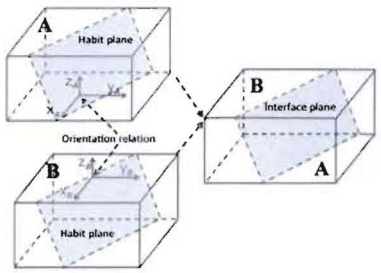


Figure 1. Variables in describing an interface: the orientation relationship (OR) between the two crystals A and B is defined using their crystallographic coordinates $(x_A,y_A,z_A)$ and $(x_B,y_B,z_B)$; interface plane is a cut-plane which is shared in both crystals; habit plane in each crystal is a plane which has the same normal as the cut-plane. When OR is given, habit planes in both crystals are related.

| Orientation Relationship | | Interface Plane | Compact Plane | Compact direction | Similarity of UC |
|---|---|---|---|---|---|
| K-S | type 5 | y-z | (No, No) | (No, No) | (No, No) |
| | type 2 | z-x | (No, No) | (Yes,Yes) | (No, No) |
| | type 1 | x-y | (Yes,Yes) | (Yes,Yes) | (No, No) |
| N-W | type 3 | y-z | (No, Yes) | (No, No) | (Yes,Yes) |
| | type 4 | z-x | (No,Yes) | (Yes,Yes) | (No, No) |
| | type 1 | x-y | (Yes,Yes) | (Yes,Yes) | (No, No) |

Table 1: Six interfaces in fcc/bcc composites. In the (*,*), the 1st term represents fcc crystal and the 2nd represents bcc crystal. The KS OR holds the relation in fcc: $x \| [\bar{1}10]$, $y \| [\bar{1}\,\bar{1}2]$, $z \| [111]$ and in bcc: $x \| [\bar{1}11]$, $y \| [1\,\bar{1}2]$, $z \| [110]$. The NW OR holds the relation in fcc: $x \| [10\bar{1}]$, $y \| [\bar{1}2\bar{1}]$, $z \| [111]$ and in bcc: $x \| [00\bar{1}]$, $y \| [\bar{1}10]$, $z \| [110]$.

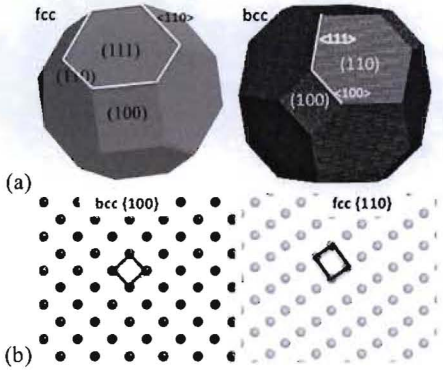


Figure 2. Compact plane, compact direction, and the similarity of atomic structures of unit cells in habit planes. For Fcc, compact planes are {111} and {100}, compact direction along <110>; for Bcc, compact planes are {110} and {100}, compact directions along <111> and <100>.

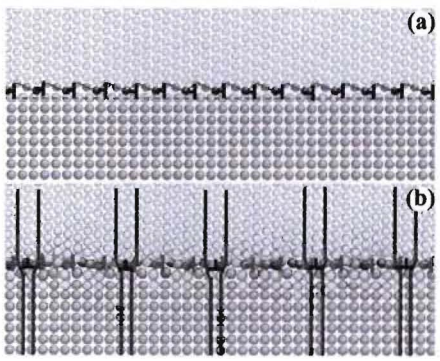


Figure 3. Atomic structures of a type-4 interface before and after relaxation. The top grain is Cu and the lower grain is Nb.

## 3. SHEAR RESPONSE OF INTERFACES

The shear strength of an interface is the critical shear stress at which irreversible sliding of one crystal with respect to the other commences along the interface. This is determined by gradually increasing a homogeneous shear strain applied to bilayer

models of Cu/Nb [5]. The in-plane shear resistance for a type-1 interface (NW:x-y) is plotted in Fig. 4b. The results revealed that the shear strength of a type-1 interface (i) is significantly lower than the theoretical estimates of shear strengths on glide planes in perfect crystals of Cu and Nb and (ii) is anisotropic (i.e., dependent on the applied in-plane shear direction). Details of the atomic-scale sliding in interfaces are revealed by disregistry analysis [1]. The same phenomena are revealed for both type-1 interfaces (KS:x-y and NW:x-y). When the applied shear stress reaches a critical value, irreversible sliding occurs nonuniformly, beginning within the coherent sites in the interface (Fig. 4c), suggesting that an interface sliding mechanism in which dislocation loops nucleate in interfaces and subsequently expand by gliding in the interface plane.

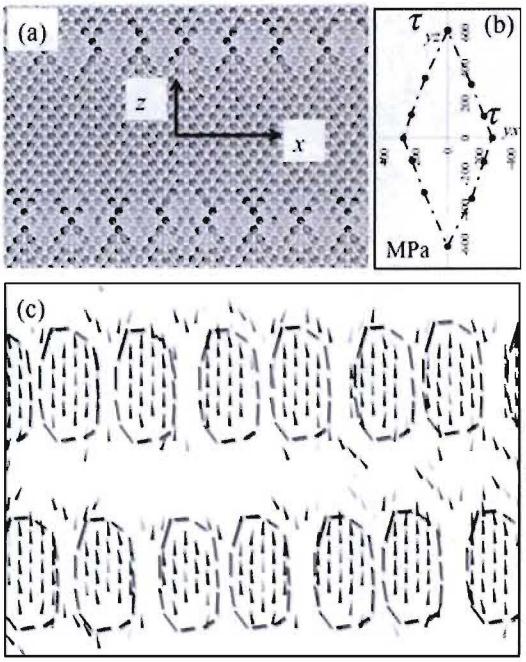


Figure 4 (a) Atomic structures of type-1 interface (NW OR), (b) the in-plane shear resistance, and (c) interface sliding mechanisms: nucleation and propagation of interface dislocation loops.

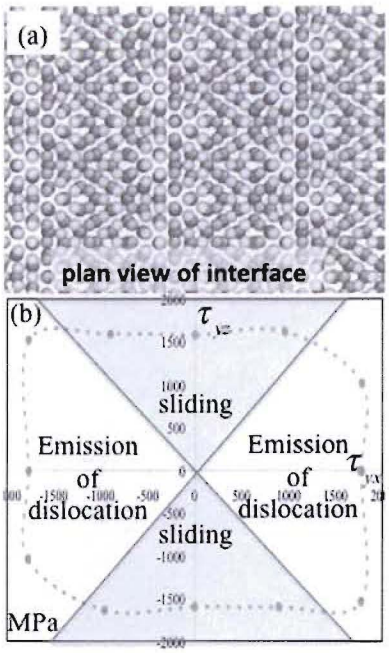


Figure 5 (a) Atomic structures of type-4 interface and (b) the in-plane shear resistance and shear response (sliding and emission of lattice dislocation).

The plan-view of the atomic structure and the in-plane shear resistance for type-4 interface is plotted in Fig. 5a and b. The results show that (1) the interface likely slides along the compact direction and (2) lattice dislocations can be emitted from interfaces due to the dissociation of interface disconnections. These two mechanisms can be associated with the interface flow strength curve as indicated in Fig. 5b. Similar results are found for type-2 interfaces. For type-3 interfaces, lattice dislocations nucleate and emit from the interface at the boundaries of coherent and incoherent regions in the interface, when the applied shear stress reaches a critical value. For type-5 interfaces, the shear response of the interface is complicated due to the disorder nature of their atomic structure, and requires further study.

## 4. DISLOCATION-INTERFACE INTERACTIONS

The interaction of lattice dislocation with the interface is strongly dependent on interface defect structures and interface shear strength. For interfaces containing interface disconnections, the interaction force between them acting on the lattice dislocation could be either attractive or repulsive depending on the character of the impinging dislocation. The reaction products left in the interface could lead to the rearrangement of the atoms within the interface in order to achieve a new low energy state.

For flat interfaces, interface shear strength is a dominant factor [6]. As a consequence of the low shear resistance of the type 1 interfaces, the interface will shear in response to the stress field of a nearby dislocation and attract the dislocation into the interface wherein the core of the dislocation spreads [1]. Using atomistic simulations, we showed that a dislocation, no matter what type or sign, spontaneously enters the interface, from Cu due to shear of the interface. The core of the lattice glide dislocation readily spreads within the Cu-Nb interface, resulting in a nonplanar core structure. The width of core spreading increases with decreasing shear strength [5]. We also studied the core spreading of lattice dislocations in Nb within interfaces, and the same study has been performed for type-1 NW interface. Similar phenomena are observed.

With respect to different shear strength, the attraction force can be derived as the first order derivative of the potential energy with respect to the distance from the interface. The change of potential energy is due to two factors, one arising from the Koehler force and the other from the sheared interface. The potential energy due to the sheared interface is determined from atomistic simulations as a function of the distance from the interface [5]. For glide dislocations in a Cu crystal, the potential energy always decreases as a glide dislocation approaches the interface [5]. For glide dislocations in an Nb crystal, the potential energy increases until a critical distance is reached, and then decreases [5]. The result reveals that the interface with the lower shear strength results in the quick drop of energy as the dislocation approaches the interface, implying the stronger attraction force on the dislocation.

## 5. SLIP TRANSMISSION OF DISLOCATION ACROSS INTERFACES

### 5.1 A Single Dislocation across fcc/bcc Interface

For the case of dislocation trapping in the interface plane via core spreading, slip transmission is achieved through three unit processes: (a) a glide dislocation is attracted into the interface in association with the core spreading within the interface, (b) the extended core has to shrink in order to nucleate a glide dislocation in the adjacent crystal, and (c) the nucleated dislocation loop bows out from the interface under stress, overcoming the attraction force due to the interface shear and the residual dislocation at interface.

For certain slip systems, the slip transmission process is studied using the chain-of-state method. First, a straight dislocation is introduced into one crystal in the bicrystal model close to the interface. After fully relaxing the dislocated configuration, the equilibrium configuration containing a lattice dislocation is

obtained, and this acts as the initial configuration. Second, the final configuration containing a dislocation loop in the adjacent crystal is created and relaxed at a certain applied stress. Finally, molecular dynamics is performed for the final configuration while reducing the applied stress to obtain a series of configurations between the initial and the final configurations. The change of potential energy is then calculated as a function of the size of the dislocation loop [1]. Corresponding to the different states, the change of potential energy of the bicrystal is calculated. The critical stress corresponding to the stabilized dislocation loop is determined from the first derivative of the potential energy with respect to the dislocation loop and found to be on the order of 0.8 GPa in terms of the resolved shear stress. Regarding different interfaces, this critical stress will increase as the interface shear resistance decreases due to the expansion of the dislocation core within the weaker interface [6].

For the case of dislocation blocking by the interface plane via the reaction with interface disconnections, slip transmission processes are complicated, involving different mechanisms, such as dislocation climb along interface, dissociation and/or recombination of interface defects, and nucleation and emission of dislocation. Correspondingly, temperature and local stresses become more important because most of these mechanisms mentioned above are thermal activated processes.

### 5.2 A Dislocation Pile-up across Grain Boundaries

Grain-boundary strengthening (or Hall-Petch strengthening) is based on the observation that grain boundaries impede dislocation movement and that the number of dislocations within a grain have an effect on how easily dislocations can traverse grain boundaries and travel from grain to grain. In grain-boundary strengthening the grain boundaries act as pinning points impeding further dislocation propagation. Since the lattice structure of adjacent grains differs in orientation, it requires more energy for a dislocation to change directions and move into the adjacent grain. The grain boundary is also much more disordered than inside the grain, which also prevents the dislocations from moving in a continuous slip plane. Even for a certain grain boundary, atomic structures or defect structures differ along the grain boundary; correspondingly, the pinning strength will vary with the location of impinging dislocations at the grain boundary.

Under an applied stress, existing dislocations and dislocations generated by Frank-Read Sources will move through a crystalline lattice until encountering a grain boundary. As more dislocations propagate to this boundary, dislocation "pile up" occurs as a cluster of dislocations are unable to move past the boundary. As dislocations generate repulsive stress fields, each successive dislocation will apply a repulsive force to the dislocation incident with the grain boundary. These repulsive forces act as a driving force to reduce the energetic barrier for dislocation across the boundary, such that an additional pile up pushes the dislocation across the grain boundary, allowing further deformation in the material.

To understand the mechanism of grain boundary strengthening one must understand the nature of dislocation-grain boundary interactions. Using atomistic simulations, we studied the effect of atomic structures of grain boundary on pinning strength associated with slip transmission across an asymmetric tilt grain boundary of Al [7]. It is observed that the grain boundary is faceted and contains an array of

interface disconnections (Fig. 6). Steps are regularly distributed along the grain boundary and interface disconnections are present at the steps. Molecular dynamics simulations are conducted at room temperature (300 K) for an Al bicrystal in which the lower grain contains 20 dislocations with Burgers vector of ½<110> on the {111} plane, forming a dislocation pile up. To reduce the shock effect, these dislocations are introduced one by one in the lower grain using a Predict—Correct method. At first, we estimate the position for a newly introduced dislocation based on linear elastic theory, then the dislocation is introduced at the predicted position by applying the displacement field of a dislocation. Second, the system is relaxed for 40 ps. The final position is determined using disregistry analysis. Third, we correct the displacement field in the fixed region of the simulation cell by introducing a dislocation dipole, the same sign dislocation is placed at the final position and the opposite sign dislocation at the predicted position. The corrected system is then relaxed again. Using the corrected and relaxed configuration as a reference, then we estimate and introduce the next dislocation in the lower grain. By repeating the above processes, a dislocation pile up can be generated at a steady state, reducing the shock effect that would accompany inserting a dislocation pile up all at once.

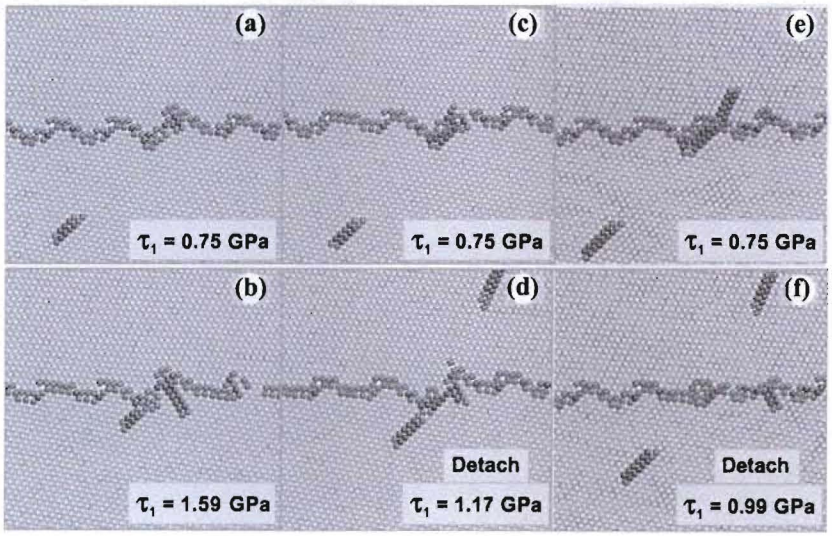


Figure 6 Atomistic structures of grain boundaries with respect to the different impinging positions. The impinging position is at the step (a) the 1st incoming dislocation at GB under the local resolved shear stress (RSS) 0.75 GPa and (b) transmission does not take place even at RSS 1.59 GPa; close to the step (c) the 1st incoming dislocation at GB under the local RSS of 0.75 GPa and (d) transmission takes place at RSS 1.17 GPa; at the middle of the flat region (e) the 1st incoming dislocation at GB under the local RSS 0.75 GPa and (f) transmission takes place even at RSS 0.99 GPa.

To explore the effect of local structures on pinning strength, we study three cases with respect to the three positions at the grain boundary [7]: one at the step (interface disconnection, Fig.6 a and b), the second at the middle between two adjacent steps (flat region, Fig. 6 e and f), and the third in-between the above two positions (Fig. 6 c and d). The results show that (1) the step plays the strongest pinning effect. Even at 1.59 GPa, the slip transmission did not take place; (2) the

flat region has the lowest pinning strength (0.99 GPa); and (3) the pinning strength at the region in-between the above two positions is 1.17 GPa. It is reasonable to conclude that the reaction between the impinging dislocation and the pre-existing interface disconnection causes a strong pinning effect due to the change of the character of the impinging dislocation.

## 6. CONCLUSIONS

Using atomic scale models, interface defect theory, and molecular dynamics simulations, we classify interface structures into five types with respect to geometric factors. Corresponding to the characteristics of the five types of interfaces, we found that interface shear response and shear mechanisms can be related to the geometric factors. For type 1 interfaces, we studied the dislocation-interface interactions and slip transmission mechanisms. The results show that type 1 interface (a weak interface with the low shear strength) attracts dislocations due to the interface shear, traps lattice dislocations due to core spreading, and as a result, impedes dislocation transmission across the interface. Take an Al GB as an example type-2 interface, the results show that pinning strength is strongly dependent on the local structure of the interfaces. The flat region has the lowest pinning strength; the reaction of interface disconnection with the lattice dislocation will change the character of the lattice dislocation, causing a stronger pinning effect.


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