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Review

# Interaction of Dislocations and Interfaces in Crystalline Heterostructures: A Review of Atomistic Studies

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**Abstract:** Interfaces in heterostructures of crystalline materials could strongly affect the slip of dislocations. Such interfaces have become one of the most popular methods to tailor material strength and ductility. This review focuses on the interaction of dislocations and interfaces in heterostructures, in which at least one component is metallic, as investigated by molecular dynamics, in order to systematically summarize our understanding about how dislocations interact with the interfaces. All the possible heterostructures of metallic materials are covered, such as twin boundaries, grain boundaries, bi-metal interfaces and metal/non-metal interfaces. Dislocations may either penetrate the interfaces by inducing steps into the interfaces or dissociate within the interfaces, depending on the type and orientation of the interface as well as the applied strain. Related dislocation interactions at the interface are also presented. In addition, we also discuss the effect of dislocation types, of applied strain and of the deformation method on the interaction of dislocations and interfaces.

**Keywords:** dislocations; heterostructures; metallic materials; twin boundaries; grain boundaries; interface; molecular dynamics

## 1. Introduction

Heterostructures are found in metallic materials including metals, alloys, multi-layer materials, coating materials and metal-matrix composites. They are induced by twin boundaries (TBs), grain boundaries (GBs), the second phase, etc. The interfaces formed are essential for changing the threshold of deformation and the motion of dislocations, and thus for optimizing the comprehensive mechanical properties as well as the strength [1–5]. The underlying mechanisms could be interpreted as the interaction of dislocations and interfaces in metallic heterostructures.

Therefore, the mechanisms regarding how dislocations interact with interfaces—including twins boundaries, GBs, bimetallic interfaces, and metal/nonmetal interfaces—have been studied intensively. It has been proved that different interfaces in metallic heterostructures interact with dislocations in a totally different manner. Thus, the related strengthening and toughening mechanisms change with the interface types of metallic materials.

For example, Lu et al. [6] observed that the yielding mechanism depends on the twin thickness and changes from the slip transfer across TBs to the activity of preexisting easy dislocation sources.

Experimentally, Li et al. found that coherent TBs can react with each other to facilitate the multiplication of partial dislocations in coherent TBs [7,8]. In the case of GBs, their interaction with lattice dislocations is the critical atomic process governing the mechanical behavior of polycrystalline metals [9,10]. Numerous studies on the slip transfer mechanisms were performed and results show: (a) direct transmission of slip, (b) direct transmission with a residual dislocation left at the GB, (c) absorption of impinging lattice dislocations and emission of new lattice dislocations at different sites from the GB, (d) incorporation of the dislocation into the GB [11–14]. When dislocations interact with the bimetallic interfaces, the dislocation transmission contributes to the formation of crystallographic bands of intense plastic strain [15]. During the indentation into Al/Nb multilayers [16], preferential storage of dislocations at interfaces, as opposed to within layers, recovers through climb in the interfaces due to high vacancy diffusivity and vacancy concentration of the interfaces.

Even though the above-mentioned experimental results display remarkable progress in the interaction of dislocations and interfaces in metallic materials, it is extremely difficult for experiments to investigate the details at the atomic scale, to illustrate the evolution of plasticity and thus to shed light on the underlying mechanisms. These goals could be reached by molecular dynamics (MD) simulation. The work of Van Swygenhoven [17] pioneered the use of MD simulations to investigate the interaction of dislocations with GBs during deformation. Later, Schiotz and Jacobson [18] discovered that the microscopic deformation mechanism in Cu features a shift from dislocation-mediated plasticity in the coarse-grained material to GB sliding in the nanocrystalline regime, leading to a maximum in the yield strength as a function of grain size.

Jin et al. investigated how coherent TBs interact with both screw lattice dislocations and non-screw lattice dislocations via MD simulations [19,20].

Using MD simulations, Salehinia et al. found that interface misfit dislocations result in the nucleation and slip of lattice dislocations in the metal layer during the deformation of metal-ceramic (Nb/NbC) multilayers [21]. The interaction of non-metal dislocations with metal/non-metal interfaces was investigated in detail via MD simulations for a Si layer coating on a Al layer [22]. It was found that the orientation of the Al/Si interface plays a dominant role in deciding whether Si dislocations penetrate the Al/Si interfaces successfully.

Since MD simulations have been extensively applied to investigate how dislocations interact with interfaces in metallic materials, this article reviews some of the most relevant contributions to the underlying mechanisms where MD simulations were used. It focuses on the interactions between dislocations and heterostructure interfaces in metallic materials and includes the following topics:

- In Section 2, TBs of metals and alloys interact with screw and non-screw lattice dislocations.
- Section 3 focuses on the interaction of dislocations with low-angle grain boundaries (LAGBs) and high-angle grain boundaries (HAGBs).
- In Section 4, the interaction of bimetal interfaces—covering coherent, semi-coherent, and incoherent interfaces—with dislocations is reviewed.
- Section 5 focuses on metal/nonmetal interfaces interacting with both metal dislocations and nonmetal dislocations.

## 2. The Interaction of Dislocations and TBs

Twinning produces the simplest heterostructure since at the two sides of the twinning boundary, the grains have exactly the same structure. Thus, the simplest case for study is given by the interaction of a dislocation with a twinning boundary. On the other hand, twinning caused by mechanical deformation, consolidation, deposition etc., has proven to be a very effective way to improve the mechanical properties of metals and alloys [6–8]. Therefore, it is highly significant to study the interaction of dislocations and TBs and then illuminate the processes how twinning boundaries affect mechanical properties [19,20].

### 2.1. Screw Dislocations Interacting with Coherent TBs

Jin et al. [19] used MD simulation to study coherent TBs in three face-centered-cubic (fcc) metals (Al, Cu and Ni) as shown in Figure 1, and applied different stresses to investigate how the dislocation/coherent TB interaction processes depend on the applied stress and on the chemical nature of the metal. When an incident screw dislocation consisting of two Shockley partials is forced into a coherent TB by an externally applied shear $\varepsilon_{appl}$, there are two modes of interaction how the dislocation may propagate into the adjacent twin grain: (i) by cutting through the boundary and (ii) by dissociating within the boundary plane. Which one of these two interaction modes applies depends on the material-dependent energy barrier for the nucleation of Shockley partial dislocations [19].

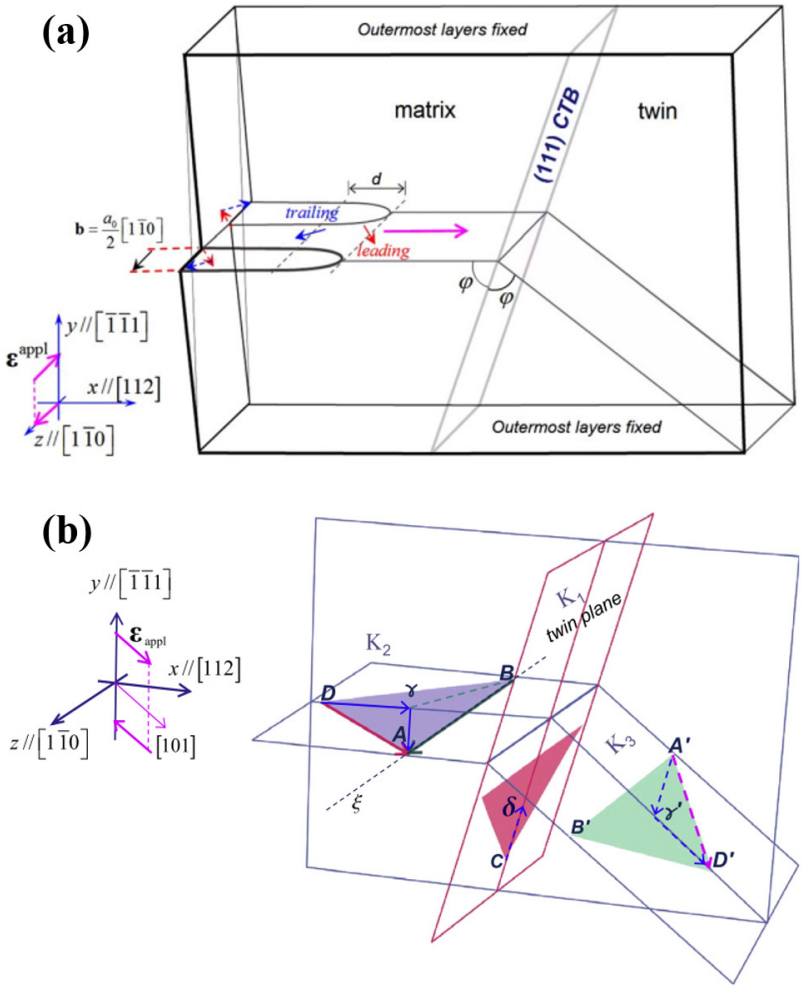


**Figure 1.** Configuration of a twinned bi-crystal for simulating the interaction between (**a**) an incident screw dislocation and (**b**) a perfect lattice dislocation with a coherent twin boundary in fcc metals. $\varepsilon_{appl}$ denotes the applied shear strain that drives the dislocation towards the twin boundary. Figures taken from Refs. [19,20] with permission.

Another MD simulation of uniaxial tensile deformation of nano-twinned Cu [23] showed that an abundance of TBs provides an obstacle to the dislocation motion, resulting in a high strain-hardening rate. Wu et al. [24] observed through MD simulations of Cu that TBs can act as both dislocation barriers and multipliers during plastic deformation. Later, MD simulations combined with experiments [25] were used to analyze the slip transfer reactions between lattice dislocations and coherent TBs, reaching similar conclusions such as dislocation absorption into the TB and slip through the TB. Also, the interaction of two different twin boundaries in Mg [26] with screw dislocations was investigated

by MD simulations. The results confirmed that screw dislocations may either be absorbed readily in the boundary or pass through the twin boundary. The mechanisms presented are similar to those in the previous studies [19,20].

In summary, screw dislocations can get stuck in coherent TBs—by dissociation into two Shockley partial dislocations with a pair of opposite moving directions—or penetrate the coherent TB completely.

### *2.2. Non-Screw Dislocations Interacting with Coherent TBs*

The scenario discussed in the previous section is limited to pure screw dislocations, where the dislocation line is parallel to the twin plane, which is a very special and simple case. To complement these universal results, the interaction between non-screw dislocations and coherent TBs in fcc metals [20] was reported in detail. It was observed that non-screw dislocations interact with the boundary in different ways: if the external stress forces a 60° dislocation into the coherent TB, it breaks down into different partial dislocations and slides into the twins and along the twin boundary. If the transmitted slip is incomplete, a sessile dislocation lock can be generated at the coherent TB, which depends on the material and the applied strain. By contrast, the energy barrier for the nucleation of Shockley partial dislocations determines how screw dislocations interact with coherent TB interactions [19].

Subsequently, Li et al. [7] proposed a dislocation multiplication mechanism on the basis of dislocation theory and MD simulations. Successive dissociation reactions can lead to a continuous dislocation source under suitable applied stress states. These observations confirmed that—in addition to acting as barriers to slip transmission—coherent TBs can react with a lattice dislocation to allow for the multiplication of partial dislocations; as a result the entire coherent TB may experience a translation.

Additionally, pre-existent defects in TBs affect the interaction of dislocations and coherent TBs, which was also studied [27]. It is found that, when the applied shear strain exceeds 1.06% in nanotwinned face-centered cubic metals, a kinked twin boundary is effective in changing the mechanism from direct dislocation transmission to dislocation absorption, which produces significant hardening [27].

Thus, besides the interactions modes found for screw dislocations, a non-screw dislocation can also be absorbed in a coherent TB partly forming a sessile dislocation lock or penetrate a coherent TB partly.

## 3. The Interaction of Dislocations and GBs

The Hall-Petch relationship [28,29] is widely used to calculate the yield strength based on the grain size of metals and alloys. According to the Hall-Petch relationship [28,29], dislocations slip and move with higher difficulty when the the density of GBs increases. Therefore, the question of how GBs interact with dislocations at the atomic level constitutes the key point to deepen our understanding of this general phenomenon. This issue can be better resolved by MD than by experiments. Van Swygenoven [17] was the first to use MD simulations to shed light on the interaction of dislocations with GBs in nanocrystalline Ni. Subsequently, Schiotz and Jacobsen [18] used this method to simulate the plastic deformation of nanocrystalline copper. They demonstrated that the microscopic deformation mechanism performs a transition from the dislocation-mediated plastic deformation in the coarse-grained material to GB slip in the nanocrystalline region, leading to a maximum in strength of nanocrystalline Cu.

Twinning is often observed during the deformation of polycrystalline metals. Therefore, for such polycrystalline metals, dislocation slip could be affected by TBs as well as GBs. The coupling effect of TBs and GBs on dislocation slip tends to be more complex, compared with that of only one factor, but could be also investigated in detail via MD simulations. Thus, Yamakov et al. [30] studied the interaction of dislocations and GBs in the room-temperature plastic deformation process of nanocrystalline Al. They showed that the interplay of dislocation and GB processes becomes stronger

with grain size decreasing to nanoscale. Unlike at nanoscale, mechanical twinning may have a weaker contribution to the deformation behavior of coarse-grained aluminum.

In the following, we separately discuss dislocation interaction with LAGBs and HAGBs. In addition, special attention is paid to the peculiarities of dislocation pile-ups interacting with GBs.

### *3.1. Dislocations Interacting with LAGBs*

The interaction of dislocations with LAGBs plays an important role in strengthening metals and could be investigated in detail via simulations. Liu et al. [31] used dislocation-dynamics simulations of a body-centered-cubic (bcc) crystal and modeled the LAGB by three sets of dislocations forming a hexagonal dislocation network. They found that when lattice dislocations approach and attempt to penetrate the LAGB, the GB can massively obstruct and even prevent dislocation transmission.

The interaction between LAGBs and dislocations of both pure screw and 60° mixed character has been studied in Ni through MD simulations [32]. The results show that the dislocation reaction and slip transfer depend on the structure of the LAGB, the nature of the incident dislocations, and the specific slip plane that enters the slip. It is found that the dislocation transfer through the LAGB is controlled by the following factors: the misorientation angle of the GB, the Burgers vector of the incident dislocation, and the exact position where the dislocation intersects the GB. Figure 2 gives an example of the penetration of a dislocation through a symmetrical Σ57 tilt GB in Ni [33].

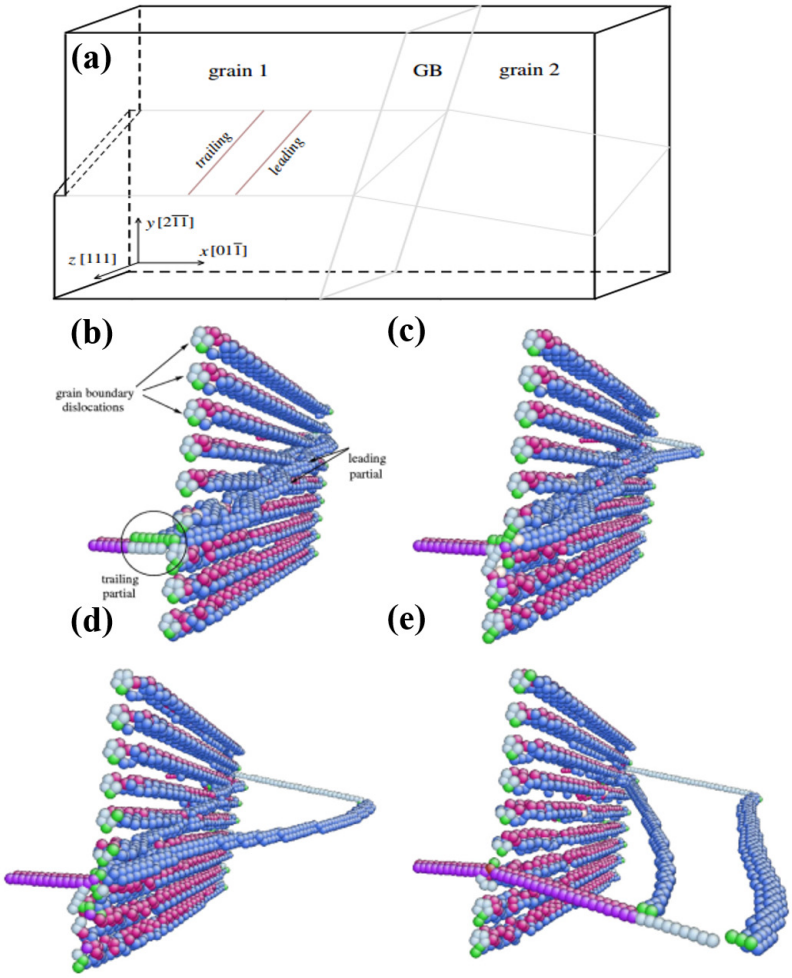


**Figure 2.** (**a**) Simulation box containing two grains misoriented around the [111] rotation axis for simulating the interaction between a lattice dislocation and a tilt GB. (**b**–**e**) Snapshots showing different steps of the interaction between a dislocation and a symmetrical Σ57 tilt GB. Figure taken from Ref. [33] with permission.

The influence of temperature on the interaction of dislocations and GBs was studied by experiments for the case of 304 stainless steel [34]. It was found that an increase of the temperature does not change the fundamental mechanisms governing slip transmission, but leads to a lower barrier for dislocation absorption and emission from the boundary and more complexity of the interactions.

In addition, dislocation nucleation is often observed at the GB [35–37]. Atomic simulation of Cu and Al under uniaxial tension perpendicular to a Σ3 GB shows [35] that dislocation nucleation at these boundaries is connected with the GB structure and energy, as well as mechanical properties of the metal. For asymmetric Σ3 boundaries in Cu [35], dislocations dissociate from the boundary and then preferentially nucleate on the maximum Schmid-factor slip plane(s) of only one grain. Dislocation nucleation is also influenced by the interface structure, stress state and initial free volume available at the GB [36]. For asymmetric twist boundaries [37], a low excess volume leads to the nucleation of a mobile GB dislocation and the motion of the GB dislocation contributes to GB sliding.

### *3.2. Dislocations Interacting with HAGBs*

MD simulations of high-angle tilt GBs in ⟨111⟩ textured thin Ni films [33] indicate that dislocation nucleation at the GB or transmission though it are difficult, since the glide planes at the two sides of the GB are highly uncorrelated. Only limited partial dislocation nucleation was observed for the HAGBs investigated in this study.

The compression of Al nanopillars containing a HAGB was studied by both MD simulations and experiments [38]. In this case, the MD simulation of an Al bicrystal with [3 4 3]/[13 $\bar{1}$7 14] orientation showed that the GB can contribute to dislocation nucleation without resulting in dislocation pile-up at the boundary.

A comparable investigation [39] of both random high-angle boundaries and a series of symmetric tilt GBs of bicrystalline nanowires was carried out in order to understand the effect of different boundary types. Both of these two types of GBs in nanowires tend to be preferred nucleation sites for dislocations and TBs, and also efficient sinks and pinning points for migrating dislocations. Some important reactions between lattice dislocations and GBs were observed in the simulations, among them the activation of a single-arm source. When dislocation cross each other and form defects, a smooth plastic behavior is found, and the mean free path of dislocation migration is reduced; however, when dislocations easily escape to the crystal surface, leading to dislocation starvation, a jerky deformation mode was predominant.

Generally, we conclude that all the GBs act as barriers to slip, leading to either direct transmission of dislocations into a neighboring grain or indirect transmission or reflection back into the original grain with an associated defect, followed by a residual Burgers vector left at the boundary. The barrier exerted by LAGBs could be overcome sometimes, leading to transmission of dislocations. However, no reports of dislocations penetrating HAGB have been found.

### *3.3. Dislocation Pile-Ups Interacting with GBs*

Multiple impact of dislocations on GBs is often relevant, leading to dislocation pile-up in front of the GB. Therefore, the long-range stress fields pose a significant problem. It could be taken into account by a multiscale framework [40–42], in which an atomistic region—modeling the cores of GBs and dislocations—is coupled to a dislocation-dynamics framework, which allows to realistically incorporate the far-ranged stress fields influencing dislocation motion and pile-up.

The results of Lee et al. [13,14,43] have already indicated that the interaction of the leading pile-up dislocation with a GB depends on the behavior of previous dislocations that reached the GB. Dewald and Curtin [40] investigated the interaction of dislocation pile-ups with Σ11–⟨113⟩ GBs in Al; they found that the main deformation mechanism is the nucleation of grain boundary dislocations (GBDs) at the intersection of dislocations and GBs. Subsequently, atomistic simulation, combined with the discrete-dislocation method, was used [41] to study screw dislocation pile-ups interacting with Σ3, Σ11 and Σ9 symmetric tilt boundaries in Al. It was found that the interaction depends on the

number of dislocations impinging and the GB geometries. Whether lattice screw dislocations transmit across the GB or dissociate into GBDs depends on the GB geometry [41]. In addition, the multiscale modeling [41] was also used to investigate dislocation–GB interactions: 60° dislocations impinging on Σ3, Σ9 and Σ11 tilt boundaries in Al. It was shown that the result of the interaction is determined more strongly by the leading partial of an incoming dislocation rather than the full Burgers vector [41].

## 4. The Interaction of Dislocations and Bi-Metal Interfaces

Nanoscale multilayer metal composites develop fast, due to their ultra-high strength, which reaches up to half of their estimated theoretical strength [44,45]. This enhancement is attributed to the presence of interfaces between two metals with different properties, such as modulus of elasticity, lattice parameters, defect energy, and slip-plane orientation [46].

Plastic deformation including the nucleation, glide, and transmission of dislocations is strongly related to the interface structure and properties [45]. Depending on the materials and orientations of the two sides, the interfaces in these systems can be divided into three broad categories: coherent, semi-coherent, and incoherent. A coherent interface is formed when the two metals have the same type of lattice structure, for example, when both metals have an fcc structure and the difference in the lattice parameters is relatively small (about a few percent). A semi-coherent interface is formed between metals having the same lattice type but having a large mismatch in the lattice parameters. This interface is characterized by a network of misfit dislocations that are requiree to accommodate the lattice mismatch at the interface. Incoherent interfaces form between materials with different lattice structures, such as fcc and bcc lattices.

Most of the metals used in multilayer systems have the same lattice type and small mismatch, and thus coherent and semi-coherent interfaces, depending on the thickness of the individual layers, can be widely observed [47–49]. However, when the thickness of a single layer exceeds a certain critical value, the coherence at the interface is lost. In addition, the strengthening mechanism in nanoscale metal multilayer systems also depends on the layer thickness, which keeps in line with the Hall-Petch effect [28,29] used in strengthening nanocrystalline materials. However, the Hall-Petch model fails, when the layer thickness falls below a few tens of nanometers. For layer thicknesses of several nanometers, the interaction between a single dislocation and an interface is the main effect in strengthening the nanoscale metal multilayer films [46].

### *4.1. The Interaction of Dislocations and Coherent Interfaces*

Shao and Medyanik [46] constructed a coherent Ni/Cu (111) interface in a bi-layer system of a top Ni layer and a bottom Cu layer; then they induced dislocations by nanoindentation into the top Ni layer in order to investigate the dislocation-interface interactions. They found that dislocations do propagate into Cu through the coherent (111) fcc interface as shown in Figure 3. However, the interface acts as a strong barrier to dislocation glide and contributes considerably to the overall strain hardening of the nanolayered material. In addition, the dislocation-interface interactions are characterized by the widening of the dissociated dislocation core at the interface and interfacial stacking-fault formation along with their effect on the material strengthening.

Previously, Rao and Hazzledine [44] had already used MD simulations to demonstrate that the multitude of interfaces in multilayered composites obstruct glissile dislocations; in the case studied, they observed a peak yield strength of multilayered Cu-Ni systems four orders of magnitude higher than for either pure Cu or Ni. Their study also presented three new effects: (i) an interface-chemical effect in which dislocations are trapped by core spreading in the interface, (ii) a coherency-chemical effect caused by coherency strains changing the effective stacking-fault energies, and (iii) a coherency-modulus effect in which coherency strains change the elastic moduli (and hence the Koehler stress) significantly.

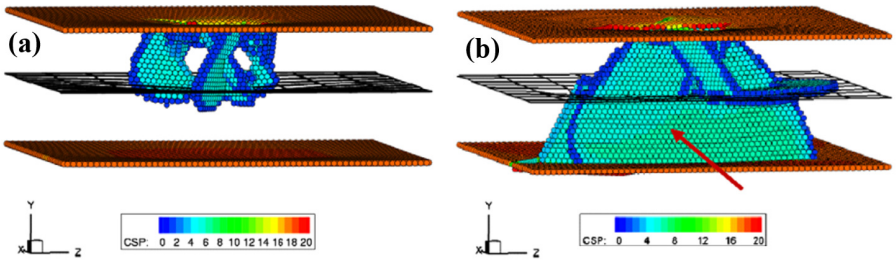


**Figure 3.** Dislocation structures developing under indention of a Ni-Cu bicrystal. Atoms are color coded according to the centrosymmetry parameter; atoms corresponding to a nearly perfect structure are not shown. Since the interface between Ni and Cu is not visible due to its coherency, a mesh that schematically represents the interface is added to the plots. At an early stage of indentation (**a**), dislocations are contained in the top Ni layer, but have traversed the interface after further indentation (**b**). The arrow points at a stacking-fault plane widening in the Cu bottom layer due to the small stacking-fault energy in Cu. Atoms are colored according to the centrosymmetry parameter. Figure taken from Ref. [46] with permission.

The misfit dislocations caused by coherent Cu-Ni interfaces was studied in detail by Hoagland et al. [50]. They found that such dislocations have very narrow cores in the plane of the interface but dissociate into Lomer-Cottrell locks out of the interface towards the Cu side. The dissociation is enhanced by the application of tensile stresses and can lead to reactions that form continuous stacking-fault structures.

### *4.2. The Interaction of Dislocations and Semi-Coherent Interfaces*

For semi-coherent interfaces, interface dislocations are required in the interface in order to alleviate the incompatibility and/or the dissimilarities between the two lattices. They act as stress annihilators to relieve the stresses away from the interfaces [51,52].

Via MD simulations combined with the classical Frank-Bilby theory, misfit dislocation structures of semi-coherent interfaces between fcc and bcc crystals were studied [45]. The results showed that there are seven sets of interface dislocations in the Nishiyama-Wassermann interface and two sets of interface dislocation in the Kurdjumov-Sachs interface. Interestingly, the interface dislocation patterns are strongly correlated with the nucleation of dislocations, including interface dislocation loops corresponding to interface sliding and lattice dislocation loops corresponding to plastic deformation in crystals.

Metals with nanoscale microstructures, such as multilayered metal composites, may show strain localization within shear bands. Their effect on the interaction of dislocations with semi-coherent interfaces was studied by Yan et al. [53] via MD simulations. The large shear stress component along the interface of the Cu/Au nanolayer, leads to a large local deformation (continuous thinning of the layer) which could unlock the products of the dislocation-interface reaction and refresh the ability of the interface to absorb incoming dislocations. This study deepens our understanding of the interface-mediated plastic deformation mechanism.

### *4.3. The Interaction of Dislocations and Incoherent Interfaces*

The incoherent interface of Cu/Nb bilayers [54] was observed via MD simulations to attract dislocations moving toward the interface. This attraction is caused by a shear of the interface induced by the stress field of the dislocation. Furthermore, upon reaching the interface, the dislocation is absorbed by it. In addition, it was also found that the resulting attractive forces on screw dislocations are larger than on edge dislocations since a screw dislocation is much more effective in shearing the interface [54].

Brittle-type failure of incoherent interfaces [55] is attributed to the limits of their ability to absorb matrix dislocations when they are opaque to dislocations and act as a dislocation sink, resulting in

shearing of the interface. An experimental study [16] of dislocation-interface interactions in Al/Nb multilayers found that dislocations are preferentially stored at the interface rather than within the layer. This study also showed that the recovery of dislocations through interface climb can be attributed to the high vacancy diffusion and vacancy concentration in the interface.

Comparing the interaction of coherent, semi-coherent, and incoherent interfaces with dislocations, we could find that the ability to absorb dislocations gradually decreases with the increase of the incompatibility. Dislocations can be dissociated at coherent interfaces, which may result in multilayers of stacking-fault structures and thus benefit the yield strength. In contrast, incoherent interfaces would appear brittle due to their high vacancy diffusion rate and vacancy concentration.

## 5. The Interaction of Dislocations and Metal/Non-Metal Interfaces

Metals usually show good ductility but low strength. The strengthening of metals could be realized efficiently by using hard non-metals to coat the surface or form composites [56]. Therefore, these coating materials and composites containing metal/non-metal interfaces possess excellent comprehensive mechanical properties and are used widely in many fields [57–59]. The mechanism of how both metal and non-metal dislocations interact with metal/non-metal interfaces constitutes the fundamental issue to understand the role of metal/non-metal interfaces in the enhancement of mechanical properties of both metallic coating materials and metal-matrix composites.

### *5.1. Interaction of Metal Dislocations and Metal/Non-Metal Interfaces*

The interface characteristics and plastic deformation mechanism of Ti/TiN multilayer systems with semi-coherent interfaces under compressive loading are studied by Yang et al. [60]. They employ MD simulations combined with the atom-informed Frank-Bilby method to characterize the interface structure and interface mismatch dislocations in the Ti/TiN system. There are three possible atomic stack interface structures based on crystallographic analysis of the interface, and misfit dislocations or dislocation nodes appear after relaxation. All the three peaks of compressive stress response of the Ti/TiN multilayer film are related to the interaction of dislocations and interfaces, including (1) the dislocation dissociation of perfect dislocation into pairs of partial dislocations around extended node regions at the interface; (2) the activation of pyramidal slip planes in the Ti layer, and (3) dislocations nucleated in or transmitted into the TiN layer.

Subsequently, Zhang and Urbassek [59] used MD simulations to study the effect of the interface shape on the interaction with dislocations. Three different shapes of the metal/non-metal interface in Al/Si composites—including particle, fiber and plate configurations—were constructed to investigate the interaction of dislocations with reinforcements of various shape during nanoindentation. The results showed that strengthening mechanisms based on the dislocation-interface interaction in metal-matrix nanocomposites depend on the shape of the reinforcements. This study confirmed that the plate interface can absorb dislocations and release them back into the matrix in a modified sliding direction, thereby reinforcing and toughening the composite, which is consistent with experimental observation [61,62].

The effect of interface structure and layer thickness on dislocation slip and the mechanical behavior of the multilayers were also studied by MD simulations of Nb/NbC multilayers [21]. In the NbC/Nb interface, there are two sets of pure edge misfit dislocations. During plastic deformation of NbC/Nb multilayers, the following mechanisms appear: (1) interface misfit dislocations lead to the nucleation and glide of metal lattice dislocations; (2) these dislocations glide in the Nb layer and are deposited at the interface; (3) the deposited dislocations facilitate slip transmission from the Nb layer to the NbC layer. The critical strain corresponding to dislocation nucleation depends on the interface dislocation structure. Furthermore, the peak flow strength of NbC/Nb multilayers is influenced by the slip transmission from Nb to NbC, the interfacial dislocations, as well as the Nb and the NbC layer thickness.

### *5.2. Interaction of Non-Metal Dislocations with Metal/Nonmetal Interfaces*

There are considerably fewer studies about the non-metal dislocations—in contrast to metal dislocations—interacting with metal/non-metal interfaces. Zhang and Urbassek [22] performed MD simulations of non-metal dislocations interacting with metal/non-metal interfaces by studying the indentation into a top layer of Si above an Al substrate. They focus on how Si dislocations impinge on the Al/Si interface and conclude that the response of Si dislocations depends entirely on the orientation of the Al/Si interface. For an interface with aligned slip systems, as shown in Figure 4, passage of the dislocations from the Si to the Al crystallite is observed, accompanied by the disappearance of the Si dislocation loops upon reaching the interface and a monolayer deep depression at the interface. The dislocations generated in Al feature large stacking-fault planes, $(1\bar{1}1)$ and (111), as can be seen in the final panel of Figure 4 at indentation depth $d = 55.2$ Å. During nucleation, $d = 54.2$ Å, three dislocations—denoted by A–C in the figure—can be observed, which are connected by the reaction A + B $\rightarrow$ C, or

$$\frac{1}{6}[1\bar{1}\bar{2}](\mathrm{A}) + \frac{1}{3}[010](\mathrm{B}) \rightarrow \frac{1}{6}[11\bar{2}](\mathrm{C})\,. \tag{1}$$

In contrast, when the slip systems of the two crystallites are not aligned, dislocation passage is strongly suppressed. When the interface consists of a close-packed plane of Al, no dislocation penetrates the interface but stacking-fault planes oriented parallel to the interface appear.

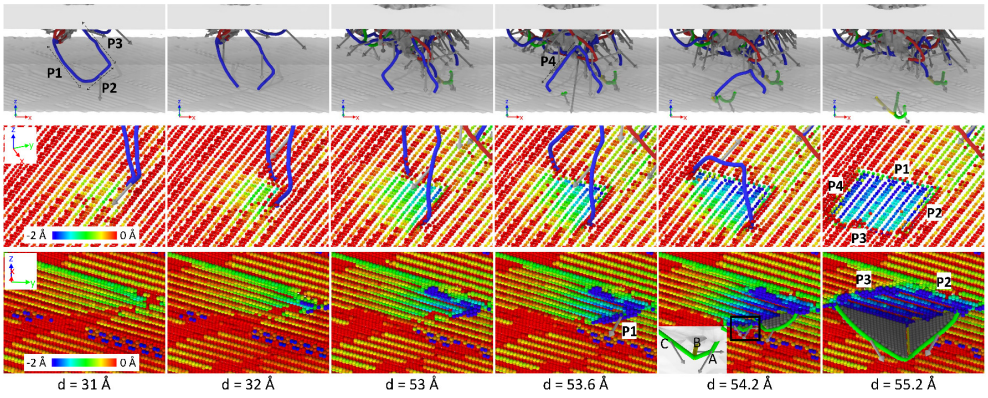


**Figure 4.** Interaction of dislocations generated by indentation of an Al/Si bicrystal to the depths $d$ indicated with the interface. Dislocations are generated in the top Si layer which is crystallographically aligned with the bottom Al layer. P1–4 denote dislocation segments. Top row: dislocations generated in the Si top layer colored according to Burgers vector: $\frac{1}{2}\langle 110\rangle$ (dark blue), $\frac{1}{6}\langle 112\rangle$ (green), $\frac{1}{3}\langle 100\rangle$ (yellow), and others (red). The gray planes indicate the surface, interface and the indent pit. Middle row: Close-up view of the penetrating dislocations and the Al interface atoms. Interface atoms are colored by height, see color bar. Bottom row: View from the Al side showing the Al interface atoms, the dislocations and the stacking faults. Insert at 54.2 Å zooms into rectangular area and demonstrates dislocation interaction, A+B=C, Equation (1). Figure taken from Ref. [22] with permission.

Via MD simulations, another phenomenon is observed in an Al/Si interface with aligned slip systems [63]. The interface is pushed toward the Al side, after a partial Si dislocation nucleates, grows through the expansion of a stacking fault, and replaces the perfect Si dislocation.

## 6. Conclusions

This review reports on important MD simulation studies of the interaction of dislocations with interfaces in metallic heterostructures including TBs, GBs, bimetal interfaces and metal/non-metal interfaces. It shows that MD simulation provides a considerable amount of crucial information on the atomic scale and is thus a promising technique to deepen our understanding of the interaction of dislocations and interfaces.

After reviewing the progress of this field, we conclude that the response of dislocations to TBs, GBs and bimetal interfaces has been investigated to a considerable extent. However, the understanding of metal/non-metal interfaces interacting with dislocations still needs to be deepened, especially on the side of non-metal dislocations. In addition, as simulation sizes are expected to become larger and larger with the ongoing development of computational facilities, it will become possible for MD simulations to investigate more complex case such as (bioinspired) nanolaminated composites [64].

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## Abbreviations

The following abbreviations are used in this manuscript:

| | |
|---|---|
| Molecular dynamics | MD |
| face-centered-cubic | fcc |
| body-centered-cubic | bcc |
| twin boundary | TB |
| grain boundary | GB |
| low-angle grain boundary | LAGB |
| high-angle grain boundary | HAGB |
| grain boundary dislocation | GBD |

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