ATOMISTIC STUDIES OF DEFORMATION MECHANISMS IN NANOSCALE MULTILAYERED METALLIC COMPOSITES

By

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ABSTRACT

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The goal of this thesis is to understand the interaction between dislocations and various metallic interfaces in nanoscale metallic multilayers (NMM). At lower strain rates, this means understanding the effect of interfaces to the strain hardening of the NMMs; at higher strain rates, this means the effect of the interfaces on the spallation strengths of the NMMs. NMMs possess ultra-high strength level which is owing to the interactions between single dislocations (i.e. no pile-up) and interfaces. In this thesis, aiming at the goal, using atomistic simulations several nanoscale metallic multilayers subjected to different loading conditions and strain rates are being considered.

First, a few simulations of nanoindentation are implemented at a low strain rate on a series of the Cu-Ni-Nb- bases metallic nanolayers. This includes the simulation of Cu-Ni and Cu-Nb bilayers, where the mechanisms of the interactions of dislocations with single interfaces are investigated in a rather isolated environment. The strengthening mechanisms of metallic multilayers are examined. Here, several types of interfaces (coherent FCC-FCC, such as Cu-Ni, incoherent FCC-BCC, such as Cu-Nb) are investigated. Several deformation mechanisms of the bilayers are
discovered. This is done Chapters two to four. Second, to address the strengthening effect of the interfaces in a more realistic, multiple interface context, a number of simulations of nanoindentations on a few Cu-Ni-Nb- based multilayers with number of interfaces up to 18 was performed. Here the surface deformation (surface pile-up) as well as the hardening behavior of the NMMs has been considered. A constitutive law addressing strain hardening in NMM under nanoindentation is developed. This is done in Chapter five. Third, to investigate the effect of the interface on the spallation strengths of the NMMs, several simulations of the NMMs under high strain rate uniaxial strains are performed. Under two different strain rates, the spallation strength ($\sigma_s$) of the NMMs and its variation with respect to the change of the individual layer thickness ($h$) are analyzed and explained. The mechanisms of the spallation in different NMMs are observed. This is done in Chapter six.
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DEDICATION

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for their selfless support during my Ph.D years and my life.
Nanoscale metallic multilayered (NMM) materials have attracted considerable research interest recently. The mechanics of deformation of these nanoscale materials differ greatly from those in macro scale. Owing to the increasing surface-to-volume ratio of materials in such a small scale, attention needs to be devoted to the presence of the interfaces. Metallic multilayers often exhibit significant increases in strength as the layer thickness is decreased from micro scale to nanoscale [1-3]. For layer thicknesses in the range of a few nanometers, the strength may be as high as one third to one half of the estimated theoretical strength [3,4]. The strength of these nano-multilayers is usually one to three times higher than the rule-of-mixtures estimate [2, 5, 6]. Normally this strength cannot be achieved by individual materials that comprise the structure. Generally, this strengthening effect is due to the presence of the interface between two dissimilar materials. Or, in other words, the strengthening can be attributed to the following four mismatches between the adjacent layers: elastic modulus, lattice parameter, gamma surface (chemical) and slip-plane [7-11].

The interfaces mentioned previously can be categorized in two different manners. According to the lattice structures and parameters of the materials on each side, the interfaces can be divided into three types: coherent, semi-coherent and incoherent. Coherent interface typically forms between two metals that have the same type of lattice structure, e.g. both face-centered cubic or both body-centered cubic, with relatively small difference between lattice parameters. At the vicinity of a coherent interface, the lattice parameter either does not change or changes gradually across the interface. Semi-coherent interface usually can be found when two materials on both sides have the same lattice type but the difference in lattice parameters is quite large, or the
mismatch between the lattice parameter is small but the thickness of each individual layer exceeds a certain threshold value [12]. In this case, the mismatch between the lattice parameters is accommodated in terms of a network of misfit dislocations at the interface [13]. Incoherent interface generally exists between two materials with different lattice types, e.g. face-centered cubic and body-centered cubic materials. This type of interface usually possesses a low shear strength compared to other type of interfaces; hence it is often referred to as weak interface.

Alternatively, according to different structures and resistance to slip transmission the interfaces can be classified into the following two families: transparent and opaque [14]. Transparent interfaces normally have the following properties. Across the interface, the slip systems are almost continuous, and, compared to the slip resistance of a bulk system, exerting a very insignificant resistance to slip. Transparent interfaces normally include coherent and semi-coherent interfaces. While for opaque interfaces, several unique characteristics apply. First, the slip systems are discontinuous across the interface, usually resulting from the change of lattice types. Second, the shear strength of the interface is quite low which attracts and absorbs dislocations. Hence, this type of interface is acts an obstacle for slip transmission.

The strengths of the nanoscale multilayered materials are very much dependent on the thickness of the individual layers. Experimental data [10, 15] shows that when individual thickness is above of about 50 nm, the hardness of multilayered materials agrees well with what is predicted by the Hall-Petch model:

\[ \sigma_y = \sigma_0 + \frac{k}{\sqrt{h}}, \]  

(1)

where the yield strength \( \sigma_y \) is inversely proportional to the square root of the individual layer thickness \( h \). It is believed by researchers that, in this scenario, the dislocation pile-up is playing
an important role in determining strength with layer thickness viewed as the distance between barriers to slip [16,17]. The strength of the system is thus determined by the applied stress which makes the stress at the tip of the pile-up sufficient for the dislocation to burst through the interface or activate the slip system on the other side of the interface. When the layer thickness is less than 50 nm, experiments show that the hardness increases with decreasing layer thickness until it reaches a peak value below about 5 nm and the Hall-Petch model breaks down. This can be explained that, as the layer thickness drops below 50 nm, there is not much room for dislocations to the pile-up. Thus the load needs to be higher for dislocations to propagate through the interfaces. At this scale, the strengthening of the nanoscale multilayers is mainly attributed to the interaction of single dislocations with the interfaces. Currently, there are several models that have been proposed to address the strength of the NMMs under such lengths scales. Using dislocation dynamics, Akasheh et al. [18-19] showed that for Cu-Ni NMMs the confined layer plasticity (CLP) is main plastic deformation mechanism and the interaction between the threading dislocations and the interfacial dislocations is responsible for the strength of the Cu-Ni NMMs. A constitutive relation has been proposed based on their findings. The work of Misra et al [11] showed that for the high strength of Cu-Nb NMMs are mainly due to the confined layer slip (CLS) and the interface crossing (slip transmission). In this work, a refined confined layer slip model has been proposed. When the individual layer thickness goes to about 1-2 nm, then a softening of strength will be observed with the decrease of the thickness. Wang et al [20] suggested that the slip transmission is the main mechanism for the strength of the NMMs at this scale. As mentioned above, although considerable amount of work has been done addressing the NMMs, the deformation of the NMMs is far from being fully understood. First, the interaction of dislocations with interfaces seems to be greatly affected by the types of the interfaces and even
by each pair of materials composing the interface. Hence, different types of interface, even the same type of interface but with different composing materials are worth being addressed separately. Second, although there are a good amount of experimental works available addressing the work hardening of the NMMs, the numerical and theoretical works addressing this issue are still scarce. Thirdly, most work currently available addressing the deformation of the NMMs are all under the low strain rate regime. It is unclear whether the mechanisms of interactions of dislocations with interfaces under high loading rates differs from that under low (quasi-static in this work) strain rates. Thus, it is necessary to investigate the mechanisms of dislocation-interface interaction as well as the strengths of the NMMs under high strain rates.

Currently, scanning probe microcopies (SPM), e.g. scanning tunneling microscopy (STM) and atomic force microscopy (AFM) have enhanced the vision of the researchers up to the atomic scale. With the aid of these technologies, one can actually see the crystallographic structure of materials. However, it is still highly impractical to monitor the development atomic structures during the process of the slow deformation not to mention that under shock loading. In the recent few decades, numerical algorithms have been developed to simulate the deformation of materials at nanoscale, e.g. molecular dynamics/statics and dislocation dynamics. Moreover, the development of high performance parallel computer also allows the simulation to be carried out on a relatively large simulation cell.

Hence, in this thesis, the plastic deformation of the NMMs under low strain rate nanoindentation will be considered. The effect of the different interfaces on the strain hardening of the NMMs will be investigated. The deformation and spallation of the NMMs under high strain rate loadings...
will also be examined. The mechanisms of the dislocations-interface interaction and spallation, as well as the spallation strengths of the NMMs will be addressed.

Recently, atomistic simulations using empirical inter-atomic potentials have been applied to study the discrete dislocations and their interaction with interfaces as well as grain boundaries for a variety of pure material and composites. Hoagland and co-workers have studied coherent (Cu-Ni), semi-coherent (Cu-Ni, Cu-Ag), and incoherent (Cu-Nb) interfaces [8-9]. These works were focused on interactions of single dislocations with intermetallic interfaces under a tensile strain loading and for Cu-Ni systems. Spearot et al. [21,22] and Capolungo et al. [23] investigated tensile deformation and dislocation nucleation from bi-crystal interfaces in copper and aluminum. Van Vliet et al. [24], Ju et al. [25] and Hasnaoui et al. [26] considered nanoindentation induced dislocation nucleation and propagation in Cu, Al, Ni and nanocrystalline Au. In these studies, different techniques have been utilized to generate dislocations in the materials, i.e. tension and nanoindentation. However, they only focused on grain boundaries in bi-crystals comprised of the same material; no interfaces between dissimilar materials have been considered. Recently, Saraev and Miller have studied nanoindentation of copper multilayers [27] as well as copper crystals with nanometer-sized nickel coatings [28]. In the former work, different numbers of $\Sigma 29$ twist grain boundaries were considered. In the latter work, they considered a bi-crystal with semi-coherent Cu-Ni $\{111\}$ interface. In that case, the mechanics of plastic deformation during indentation was dominated by the misfit dislocation networks and strongly depended on the initial position of the indenter with respect to the misfits.

All of the aforementioned studies either focused on interaction of single “artificially embedded” dislocation with interfaces subjected rather simple uniaxial tensile loading, or on the interaction
of dislocations generated by nanoindentation with grain boundaries and semi coherent interfaces. However, to the author’s knowledge, certain types of interfaces, e.g. coherent FCC-FCC and incoherent FCC-BCC interfaces, had not been considered using nanoindentation in the previous simulational works. Nanoindentation is essentially a three dimensional loading technique, where a non-uniform stress distribution is exerted by the indenter. This allows the analysis of dislocation-interface interaction to be carried out in a more realistic context. Hence, in this thesis the Cu-Ni-Nb- based NMMs, specifically the CuNi, CuNb, CuNiNb, will be selected as the test subjects; and nanoindentation is used to study the interaction between dislocation and interface and the strengthening effect of the interfaces.

First, the interaction of dislocations with single interfaces needs to be considered. Thus, in the Chapters two to four, simulations of indentation are carried out on Cu-Ni (with coherent interface) and Cu-Nb (with incoherent interface) bilayers. To fully analyze the interaction, both sides of the bilayers are indented independently to let the dislocation propagate from each side of the interfaces. The effects of the different types of single interfaces on the propagation of dislocations have been closely observed. The mechanisms of the dislocation interface interaction have been studied. Second, the dislocation-interface interactions needs to be put in a more realistic context where multiple interfaces are present in the same computational structure, and a mathematical model for the strength of the NMM needs to be constructed. Hence, in Chapter five, several multilayer models, including Cu-Ni, Cu-Nb and Cu-Ni-Nb NMMs will be considered, with various individual layer thickness and indenter radius. A constitutive model describing the hardness of the NMMs under nanoindentation is proposed. Another interesting problem to note in the nanoindentation is surface pile-up phenomenon. It is discovered that the higher the pile-up, the less the strengthening is [29]. In fact, the hardening effect of the previous three types of
multilayers falls into the falling ranking (from largest to smallest), Cu-Ni-Nb, Cu-Nb, Cu-Ni. The underlying mechanism for this relation has not yet been fully understood. In Chapter five, using the multilayer models, this issue will also be addressed.

On the other hand, to address the materials subjected to high strain rate deformations, experimentally the shockwave is commonly generated using the Hopkinson bar [30] or the high power laser [31]. The highest strain rate that can be achieved in an experiment is about $10^7$ s$^{-1}$. The numerical simulation is also a common way to address the problem mentioned above. They can achieve a strain rate of up to $10^9-10^{10}$ s$^{-1}$, and can also provide a valuable insight to the mechanisms of the deformation and/or damage of materials under such high strain rates on a nano or atomics scale. MD is proven to be an effective tool to solve this type of problem [32]. Recently, a number of numerical studies on a series of different materials under shock wave loading have been conducted. The subject materials include single crystal and nanocrystalline Cu, single crystal Ni, Ni-Al nanolayers, silica glass, Cu and Zr based metallic glass, etc [33-44]. The dynamics responses of the materials, including plasticity, melting, spalling, alloying, etc, have been documented. However, to the author’s knowledge, the behaviors of nanoscale metallic multilayers, especially those with different types of interfaces, subjected to shock loadings are seldomly reported. In this sense, in Chapter six, using Cu-Ni, Cu-Nb and Cu-Ni-Nb multilayer models, the dynamic response of the multilayers under high strain rate loading will be addressed and the effect of interfaces on the materials’ overall response will be analyzed in detail. The spallation strengths of such NMMs will be obtained. The mechanisms of spallation in each type of NMMs are carefully observed and summarized. Baring such knowledge, the variations of the spallation strength with respect to the individual layer thickness under the different strain rates are analyzed and explained.
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CHAPTER TWO: STRENGTHENING EFFECT OF COHERENT INTERFACES IN NANOSCALE METALLIC BILAYERS

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Abstract

Dislocation nucleation and propagation in a Cu-Ni bilayer with coherent (111) interface are examined using atomistic simulations. Nanoindentation model is applied to generate dislocations at and near the surface. Mechanisms of interactions between gliding dislocations and coherent interface are investigated. It is found that the interface acts as a strong barrier to dislocation propagation, which results in considerable strengthening of the bilayer. The results are compared to indentation of pure Cu and pure Ni single crystals. It is found that the obtained maximum load for indentation of the Cu-Ni bilayer is higher than for any of the two pure materials. Strain hardening of the bilayer system due to the presence of interface is investigated by analyzing the indentation load-displacement curves.

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Keywords: Atomistic simulation; Molecular statics; Interfaces; Metallic multilayers; Dislocations; Nanoindentation; Nanomaterials
2.1 Introduction

The mechanics of deformation at the nano scale differs significantly from what is typically observed on the macro scale. At such a small scale, due to increased surface-to-volume ratios presence of surfaces and interfaces becomes especially important. As a result, when the layer thickness reduces to the nanometer scale, multilayered materials often exhibit unique mechanical properties, such as ultra-high strength [1–3]. Thus, nanoscale multilayered metallic materials exhibit strength levels up to one half of their estimated theoretical strength [3,4], which is significantly higher than the strength of the individual materials that compose the structure. Commonly, this strengthening has been attributed to the presence of interfaces between dissimilar materials that have a mismatch in various properties, such as elastic modulus, lattice parameter, dislocation core energy, and slip plane orientations [5–9].

Depending on the materials comprising metallic multilayers, interfaces in these systems may be generally classified into three major categories. Coherent interfaces form when the two metals at the interface have the same type of lattice structure, e.g., both face-centered cubic (FCC), and the difference in the lattice parameter is relatively small (on the order of a few percent). Semi-coherent interfaces occur when the type of the lattice is the same, but the mismatch in the lattice parameter is larger. In this case, networks of misfit dislocations form at the interface to accommodate the mismatch. Finally, incoherent (also called weak) interfaces form between materials with different lattice structures, such as, e.g., FCC and BCC (body-centered cubic). It has to be noted that in most systems comprised of materials with the same lattice structure (e.g., FCC-FCC) and a small mismatch in the lattice parameter, both coherent and semi-coherent interfaces may form. In this case, the occurrence of a particular type of interface strongly depends on the thickness of the individual layers comprising the multilayered
structure. Loss of coherency occurs when individual layer thickness exceeds some critical value; this phenomenon has been theoretically analyzed by Hirth and Feng [10]. Generally, the mechanical properties of nanoscale metallic multilayers strongly depend on the type of interfaces between the layers comprising the system.

The mechanical properties of nanoscale metallic multilayers also strongly depend on the individual layer thickness. However, this dependence is not completely understood yet. A Hall-Petch effect [11,12], which is based on the dislocation pile-up mechanisms, is considered to be the main contributor to the strengthening of nanoscale crystalline materials. However, the Hall-Petch model breaks down when individual layer thickness in multilayered systems drops below several tens of nanometers. In that case the strength still continues to increase before it reaches a plateau and then drops in most cases as the layer thickness reduces to one or two nanometers [8,9]. A major role in strengthening of the nanoscale metallic multilayers when the layer thickness is on the order of just several nanometers is attributed to the mechanisms of interactions of single dislocations with interfaces.

Atomistic simulations using empirical inter-atomic potentials have been applied to study discrete dislocations and their interaction with grain boundaries and interfaces for a number of pure metallic materials as well as composites. Thus, Hoagland and co-workers have studied coherent (Cu-Ni), semi-coherent (Cu-Ni, Cu-Ag), and incoherent (Cu-Nb) interfaces [6,7]. That work was focused on interactions of single dislocations with interfaces under a tensile strain loading and for Cu-Ni systems only cube-on-cube multi-layers with \{100\} FCC interface planes were considered. Spearot et al. [13-14] and Capolungo et al. [15] investigated tensile deformation and dislocation nucleation from bi-crystal interfaces in copper and aluminum. These
studies focused on the interfaces and grain boundaries in bi-crystals comprised of the same material; no interfaces between dissimilar materials have been considered. Recently, Saraev and Miller have studied nanoindentation of copper multilayers [16] as well as copper crystals with nanometer-sized nickel coatings [17]. In the latter work, they considered a bi-crystal with semi-coherent Cu-Ni \{111\} interface. In that case, the mechanics of plastic deformation during indentation was dominated by the misfit dislocation networks and strongly depended on the initial position of the indenter with respect to the misfits.

In this work, we study nanoindentation of a Cu-Ni bilayer with a coherent (111) interface and focus on the effects of the interface on dislocation propagation. It is especially important to study coherent Cu-Ni interfaces because recently manufactured Cu- and Ni- based nanoscale multilayered composites often have layer thicknesses on the order of just a few nanometers when coherent interfaces are more likely to form. We employ nanoindentation model in order to repeatedly generate dislocations at and near the surface and observe their evolution into the bilayer’s volume. This approach allows to investigate mechanisms of dislocation-interface interaction. In addition, the obtained load-displacement curves help to explore the overall hardening behavior and quantify the strengthening effects of interfaces.

2.2 Computational details

In this work, we perform molecular mechanics simulations using the embedded-atom method (EAM) [18,19] to model interatomic interactions. In the EAM, the total energy of a system of atoms is given as

\[ E_{tot} = \sum_i F_i(\rho_i) + \frac{1}{2} \sum_{i\neq j} \phi_g(R_{ij}) \]  

(1)
where $F_i$ is the embedding energy which is a function of the atomic electron density $\rho_i$ at atom site $i$, $\phi_{ij}$ is a pair potential interaction, and $R_i$ is a distance between atoms $i$ and $j$. The particular form of the EAM potential utilized in this work is of the type given by Voter and Chen [20,21]. The molecular mechanics simulations employ conjugate gradient procedure for energy minimization and are performed using parallel atomistic simulation program LAMMPS [22,23].

In order to study lattice defects in general and dislocation nucleation and propagation in particular we need to reliably locate those defects within the crystal structure. Several different approaches have been commonly used for this purpose based on different criteria, such as, e.g., atomic excess energy or coordination number. In this work, we employ a centro-symmetry parameter, $P$, introduced by Kelchner et al. [24]. In a perfect FCC crystal, each atom has twelve nearest neighbors. These neighbors can be divided into six pairs that have the opposite positions relative to the given atom. Based on this, the centro-symmetry parameter for a given atom is defined as follows:

$$P = \sum_{i=1,6} |\mathbf{R}_i + \mathbf{R}_{i+6}|^2$$

(2)

where $\mathbf{R}_i$ and $\mathbf{R}_{i+6}$ are the vectors that correspond to the pairs of the opposite nearest neighbors. A centro-symmetric material, such as FCC metal, tends to preserve its centro-symmetry under homogeneous elastic deformation. Thus, if the material deformation is nearly homogeneous, the value of $P$ is close to zero. However, if the material has defects present where its centro-symmetry is destroyed, $P$ will no longer be zero for the atoms comprising the defects. Instead, the parameter will have a value within the range that corresponds to a particular defect. Thus,
values of the centro-symmetry parameter for atoms comprising partial dislocation loops and stacking faults are about 1.6 and 6.4 correspondingly.

2.3 Results
The simulated Cu-Ni bilayer is shown in Fig. 1. The dimensions of the modeled atomistic domain are 172 x 60 x 172 Å. The interface between the two materials is parallel to $x - z$ plane. Fixed boundary conditions are applied in the lateral ($x$ and $z$) directions while free boundary conditions are used for the top and bottom sides of the domain. A nearly rigid spherical indenter with radius 40 Å modeled using quadratic repulsive force is applied to the center of the top surface. At each step, the indenter is lowered by 0.1 Å and equilibrium configuration is found using energy minimization. The steps are repeated until the total indentation depth reaches 14 Å.

The misfit between nickel and copper FCC lattices is approximately 2.7 %. In order to accommodate this misfit and obtain a coherent Cu-Ni interface, coherency strains have to be applied to both copper and nickel layers. Strains $\varepsilon_{xx} = \varepsilon_{zz} = -0.01384$ were applied to copper layer and $\varepsilon_{xx} = \varepsilon_{zz} = 0.01278$ to nickel layer. The resulting coherency stresses $\sigma_{xx}$ and $\sigma_{zz}$ in the center of each layer were equal in magnitude to 4.54 GPa (compressive in copper and tensile in nickel); all other components of stress were several orders of magnitude smaller. These values of coherency stresses are considerably higher than those previously found for {100} Cu-Ni interface, which were 2.38 GPa [6]. Such difference may be explained by the fact that {111} interface planes have the highest atomic density. In fact, the coherency stresses estimated based on anisotropic linear elasticity [25] are about 4.3 GPa, which is reasonably close to the values obtained in the simulation. The difference from the theoretically predicted values may be due to nonlinearity of deformation as well as surface stresses that are not accounted for in continuum elasticity theory. In the modeled bilayer, the individual layer thickness is about 3 nm. In order to
verify that it is lower than the critical value at which loss of coherency at the interface may occur, a test was performed by relaxing the system with all free boundary conditions. Even though after relaxation the bilayer was deformed due to surface stresses, no loss of coherency was observed at the interface.

The obtained load-displacement curve for indentation of the Cu-Ni bilayer is shown in Fig. 2. Here, a number of points of interest are marked with numbers (1-10) and letters (a-h). Snapshots of the atomistic domain configurations corresponding to the lettered points are shown in the corresponding pictures in Fig. 3. In these plots, atoms are color coded according to the value of centro-symmetry parameter and atoms corresponding to a nearly perfect structure are not shown. Since the interface between Cu and Ni is not visible due to its coherency, a mesh that schematically represents the interface was added to the plots.

At the first stage of the indentation process (until point 1 in Fig.2) the material deforms elastically. First inelastic response is observed at point 1 when a pair of small stacking faults form right under the indenter in (111) plane. However, this type of deformation is usually recoverable upon unloading. First considerable permanent plastic deformation occurs at the indentation depth of 7 Å (point 2 in Fig.2) when a burst of gliding dislocations occurs under indenter. A pair of leading partial dislocations nucleate near the surface, glide along {111} planes propagating through the whole Cu layer and stop at the Cu-Ni interface. Snapshots of atomistic configuration before and after this event are shown in Figs. 3 (a), (b). Here, partial dislocations (blue atoms) are shown bounding the stacking faults (green atoms). Both dislocations stop right after crossing the interface. The dislocation lines are clearly aligned along
the interface plane and have noticeable kinks where they intersect the interface; one such kink is marked with an arrow in Fig. 3 (b).

As the loading continues between points 3 and 4, new leading partials nucleate and similarly to the previous ones propagate through copper and stop at the interface (see Fig. 3(c)). The next considerable force drop (between points 4 and 5) is associated with new leading partials reaching the interface. One notable detail is that the previously existing dislocations that have bowed into the nickel layer did retract to the interface. In Fig. 3 (d), all the dislocation lines are almost perfectly aligned with the interface, except for one which has a kink marked with an arrow. A similar process occurs at the next force drop (between points 6 and 7). The interface clearly serves as a serious barrier to dislocation propagation, so that nucleating new dislocations is more favorable energetically than pushing the existing dislocations through this barrier. No dislocations can break through the interface until the indentation depth of 11.1 Å. Only at point 8 does the first partial dislocation reach the bottom free surface as demonstrated in Fig. 3(g). The indentation force reaches maximum value of 233 eV/Å at depth 13.4 Å (point 9) and drops to point 10. By this moment, a few more dislocations break through the interface and reach the bottom free surface while newly nucleated partials continue to get stuck at the interface as shown in Fig. 3 (h).

In order to investigate the influence of interface on indentation of the Cu-Ni bilayer, we performed simulations of indentation into pure Cu and pure Ni. The domain size for simulation of pure materials was equal to the whole domain size of the bilayer. A comparison of the load-displacement curves for the three cases is shown in Fig. 4. Since Ni is much harder than Cu, the Ni curve is the steepest in the elastic range, the pure Cu shows the softest response and Cu-Ni is
in the middle (though closer to Cu since we indent from the Cu side). Plastic deformation initiates in Ni and Cu at the same depth of 6.6 Å with force values 202 eV/Å and 128 eV/Å correspondingly. The maximum force values for the pure materials are 226 eV/Å at depth 12.1 Å for nickel and 152 eV/Å at 13.3 Å for copper. It is notable that the maximum force value for Cu-Ni bilayer (233 eV/Å) is not only larger than that for copper (which would be expected), but also higher than the maximum force value for nickel. Cu-Ni bilayer exhibits much more hardening in the plastic deformation range than any of the two pure materials. This remarkable hardening behavior may be attributed almost entirely to the presence of interface.

Here we have to discuss the importance of the imposed boundary conditions for this study. In many atomistic simulations of nanoindentation, a different combination of boundary conditions is usually applied – periodic at the lateral sides and fixed at the bottom. In that case, the fixed bottom may severely affect the results as dislocations would inevitably stop near the bottom creating pile-ups and imposing stresses on the new gliding dislocations. In some cases these undesirable affects may be alleviated by increasing the simulation box size (as, e.g., in [17]). However, in the case when multilayered systems are investigated with layer thicknesses on the order of just a few nanometers, considerable stresses due to dislocations stuck at the bottom may extend well up to the interfaces between the layers and affect the dislocation-interface interactions.

The combination of boundary conditions (free bottom and fixed lateral sides) chosen in the current work allows to isolate the effect of interface. Even though the fixed lateral sides still impose certain limitations on the movement of dislocations, the domain was chosen wide enough to considerably alleviate these limitations. Most dislocations that nucleate under the indenter can
glide along the slip planes and reach the free bottom before they hit the fixed lateral boundaries. As a result, we can be sure that most of the system’s stiffening observed from the force-displacement curves in Fig. 4 comes not from the fixed boundaries but from other mechanisms, such as materials hardening due to dislocation-interface interactions.

One interesting observation may be made if we connect by a straight line two special points on each of the three curves shown in Fig. 4. In each case, the first point corresponds to initiation of plastic deformation while the second corresponds to the maximum observed force value. The slope of this line is equal to 3.586 eV/Å² for copper, 4.36 eV/Å² for nickel, and 12.629 eV/Å² for Cu-Ni bilayer. Thus, the slope values are approximately equal for the two pure materials while the value corresponding to the bilayer is about three times larger. The only possible reason for such a big difference is the presence of interface in the bilayer. This can be seen as a clear indication of the strengthening effect of interface.

2.4 Conclusion

Nucleation and propagation of dislocations in a Cu-Ni bilayer with coherent (111) interface during nanoindentation have been studied using atomistic simulations. Dislocation-interface interaction mechanisms have been investigated. It was found that even though dislocations eventually do propagate through the whole bilayer, interface acts as a strong barrier to dislocation propagation. The dislocation-interface interactions result in the overall strengthening of the metallic bilayer. The strengthening effect of the interface has been isolated by applying a particular combination of boundary conditions. Furthermore, the strengthening effect has been identified by comparing to the indentation of similar size systems comprised of pure Cu and pure Ni. The maximum load for indentation of the Cu-Ni bilayer was higher than that for any of the two pure materials. Strain hardening in the three systems (one bilayer and two
single crystals) has been analyzed based on the indentation load-displacement curves. It has to be noted that the slopes of the lines utilized for this analysis represent a convenient measure that helps to estimate how dislocation-interface interaction can manifest itself in a macroscopic plastic response. However, further work is needed in order to establish a proper connection between this measure and macroscopic hardening behavior of materials. Furthermore, analysis of the indentation of Cu-Ni bilayers with indenter applied to the Ni side, when dislocations propagate from nickel into copper, as well as work on the indentation of Cu-Nb bilayers with incoherent interface are currently underway [26].

Acknowledgments

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References

Figure 2.1 Initial configuration for a Cu-Ni bilayer. Top layer (red) is copper, bottom layer (blue) is nickel. The interface is FCC (111) plane for both materials.

Figure 2.2 Load-displacement curve for indentation of Cu-Ni bilayer. Snapshots of the atomistic configurations corresponding to the points marked with letters (a-h) are shown in Fig. 3.
Figure 2.3 Atomistic configuration at several stages of indentation. Atoms are color coded according to the value of centro-symmetry parameter. Mesh shows the interface.
Figure 2.4 A comparison of load-displacement curves for indentation of the Cu-Ni bilayer, pure Cu, and pure Ni.
CHAPTER THREE: DISLOCATION-INTERFACE INTERACTION IN NANOSCALE FCC METALLIC BILAYERS

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Abstract

Dislocation-interface interactions are investigated in a Ni-Cu bilayer using molecular mechanics simulations. Nanoindentation model is used to generate dislocations in the top Ni layer and study their propagation through coherent (111) fcc interface into Cu. Although dislocations do propagate through, the interface acts as a strong barrier to gliding dislocations and contributes considerably to the overall strain hardening of the nanolayered material. Mechanisms of dislocation-interface interactions are analyzed. In particular, spreading of a dissociated dislocation core at the interface and interfacial stacking fault formation are investigated along with their effect on the material strengthening.

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Keywords: Nanomaterials; Metallic composites; Interfaces; Dislocations; Atomistic simulation; Nanoindentation

3.1 Introduction

Nanostructured materials often exhibit unique mechanical and physical properties in comparison to their macro-scale counterparts. Thus, nanoscale multilayered metallic composites have been shown to possess ultra-high strengths, up to one-half of their estimated theoretical strength (Misra and Kung, 2001; Misra et al., 2004). This strengthening has been attributed to the presence of interfaces between metals that differ in various properties, such as, e.g., elastic modulus, lattice parameter, defect energies, and slip plane orientations (Rao and Hazzledine, 2000; Hoagland et al., 2002; Hoagland et al., 2006; Misra et al., 2002; Misra et al., 2005). Depending on the materials comprising metallic multilayers, interfaces in these systems may be classified into three major categories: coherent, semi-coherent, and incoherent. Coherent interfaces form when the two metals have the same type of lattice structure, e.g., both face-centered cubic (fcc) and the difference in the lattice parameter is relatively small, on the order of a few percent. Semi-coherent interfaces form between metals with the same lattice type but larger mismatch in the lattice parameter. Such interfaces are characterized by networks of misfit dislocations that are needed in order to accommodate the lattice mismatch at the interface. Incoherent interfaces form between materials with different lattice structures, e.g., fcc and bcc (body-centered cubic).

In most multilayers comprised of metals with the same lattice type and a small mismatch both coherent and semi-coherent interfaces may form depending on the thickness of the individual layers. In this case, loss of coherency at the interface occurs when the individual layer
thickness exceeds some critical value (Hirth and Feng, 1990). Furthermore, strengthening mechanisms in nanoscale metallic multilayers also depend on the layer thickness. Thus, a Hall-Petch effect that is considered to be the main contributor to strengthening of nano-crystalline materials is based on the dislocation pile-up mechanisms. However, the Hall-Petch model breaks down when the layer thickness drops below several tens of nanometers. A major role in strengthening of the nanoscale metallic multilayers when the layer thickness is on the order of just several nanometers is attributed to interactions between single dislocations and interfaces.

Mechanisms of interactions between single dislocations and interfaces may be fully understood only through atomistic simulation methods that allow for a detailed analysis at the atomic scale level. Atomistic simulations using empirical interatomic potentials have been applied by a number of researchers to study discrete dislocations and their interactions with grain boundaries and interfaces (see, e.g., Spearot et al., 2005; Capolungo et al., 2007; Saraev and Miller, 2005). However, most of these studies focused on interfaces and grain boundaries in bicrystals comprised of the same material. A few researchers have considered interfaces between dissimilar materials, including Cu and Ni. Thus, Hoagland et al. (2002) have studied both coherent and semi-coherent Cu-Ni interfaces. Their work focused on interactions between single dislocations and interfaces under tensile strain loading of cube-on-cube multilayeres with \{100\} fcc interface planes. Recently, Saraev and Miller (2006) studied nanoindentation of copper crystals with nanometer-sized nickel coatings. They considered semi-coherent Cu-Ni \{111\} interfaces and found that mechanics of plastic deformation during indentation was strongly dominated by the networks of misfit dislocations. However, it is also important to study coherent Cu-Ni interfaces because currently manufactured Cu-Ni multilayered composites often have
layer thicknesses on the order of just a few nanometers. In such cases, coherent interfaces are more favorable energetically than semi-coherent ones.

Medyanik and Shao (2008) have recently modeled indentation of a Cu-Ni bilayer with coherent (111) interface and analyzed the effects of dislocation-interface interaction on the overall strengthening of the material. The emphasis of that work was on identifying and quantifying the strain hardening resulting from the presence of interface and no particular mechanisms of dislocation-interface interaction have been investigated. Furthermore, in that work only dislocation nucleation in Cu and propagation through the interface from Cu into Ni was considered. In that case, dislocation propagation through the interface was rather straightforward. However, later studies by the authors have revealed considerable differences in the mechanisms of dislocation-interface interaction for the case when dislocations propagate through the interface in the opposite direction, i.e. from Ni into Cu. The results of this latest work are reported in the current manuscript. Since deformation behavior of multilayered metallic composites equally depends on dislocation movement through interfaces in both directions, it is necessary to thoroughly explore both cases. In this work, we perform atomistic simulations of nanoindentation of a Ni-Cu bilayer with coherent (111) fcc interface and focus on the mechanisms of dislocation propagation through the interface from Ni into Cu and their effect on the overall strengthening of the nanoscale metallic bi-layer.

3.2 Numerical method and computational details

Molecular mechanics simulations are performed using LAMMPS – a Sandia developed parallel atomistic simulation program (Plimpton, 1995). Interatomic interactions are modeled
using the embedded-atom method (EAM) (Daw and Baskes, 1984; Daw et al., 1993). A particular form of the EAM potential utilized in this work is of the type given by Voter and Chen (Voter and Chen, 1987; Voter, 1994). In the EAM potential, the total energy of a system of atoms is

$$E_{tot} = \sum_i F_i(\rho_i) + \frac{1}{2} \sum_{i \neq j} \phi_{ij}(R_{ij}),$$  \hspace{1cm} (1)

where $F_i$ is the embedding energy which is a function of the atomic electron density $\rho_i$ at atom site $i$, $\phi_{ij}$ is a pair potential interaction, $R_i$ is a distance between atoms $i$ and $j$, and summation in (1) is performed over all the atoms in the system.

For visualization of defects, we employ a centro-symmetry parameter, $P$, introduced by Kelchner et al. (1998). The centro-symmetry parameter for a given atom is defined as

$$P = \sum_{i=1,6} |\mathbf{R}_i + \mathbf{R}_{i+6}|^2,$$

where $\mathbf{R}_i$ and $\mathbf{R}_{i+6}$ are the vectors that correspond to the pairs of the opposite nearest neighbors of the given atom in a centro-symmetric lattice structure. A centro-symmetric material, such as fcc metal, tends to preserve its centro-symmetry under homogeneous elastic deformation. If deformation is purely elastic and nearly homogeneous, the value of $P$ is close to zero. However, if the material has defects present and its centro-symmetry is violated, $P$ will be larger than zero for the atoms comprising the defects and will have a value within the range that corresponds to a particular defect.

3.3 Simulation of nanoindentation
The initial atomistic configuration for the Ni-Cu bilayer is shown in Fig. 1. The dimensions of the modeled atomistic domain are approximately 172 x 60 x 172 Å. The interface between the two materials is parallel to $x - z$ plane. Fixed boundary conditions are applied in the lateral ($x$ and $z$) directions while free boundary conditions are used for the top and bottom sides of the domain. This combination of boundary conditions is utilized in order to allow for dislocation propagation through the whole thickness of the bi-layer and thus isolate the effect of interface on the material strengthening. Indentation is performed using a nearly rigid spherical indenter with radius 40 Å applied to the center of the top surface. At each step, the indenter is lowered by 0.1 Å and equilibrium configuration is found using energy minimization. The steps are repeated until the total indentation depth reaches 14 Å.

Preliminary analysis is necessary in order to create a coherent interface between the two materials. Thus, a lattice constant misfit between nickel and copper is approximately 2.7%. In order to accommodate this misfit and obtain a coherent Cu-Ni interface, the following strains have been applied to both layers: $\varepsilon_{xx} = \varepsilon_{zz} = -0.01384$ to copper layer and $\varepsilon_{xx} = \varepsilon_{zz} = 0.01278$ to nickel layer. These strains result in coherency stresses $\sigma_{xx}$ and $\sigma_{zz}$ that are compressive in copper and tensile in nickel and have a magnitude of 4.54 GPa in the center of each layer. These coherency stresses are reasonably close to the value of 4.3 GPa estimated based on anisotropic linear elasticity (Hirth and Lothe, 1992).

The load-displacement curve obtained from indentation of the bilayer is shown in Fig. 2. Snapshots of several atomistic domain configurations at different stages of the indentation process are shown in Figs. 3 and 4. In those figures, atoms are color coded according to the value of centro-symmetry parameter and 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.

The material initially deforms elastically, up until point 1 on the load-displacement curve. Plastic deformation initiates at the indentation depth of 5.6 Å when a burst of dislocations occurs under the indenter that results in the force drop between points 1 and 2. Initiation of plastic deformation is shown in Figs. 3a and 3b, where atomistic configurations corresponding to points 1 and 2 on the load-displacement curve are pictured. Several dislocations nucleate in Ni layer near the surface along {111} slip planes and propagate till the interface. In Fig. 3b, partial dislocation loops (dark blue atoms) are bounding the stacking faults (light blue atoms). It can be seen that dislocations get stuck at the interface and create a complex entangled structure in the Ni layer.

Atomistic configurations corresponding to points 3, 3a, 3b, 4, 5 and 6 on the load displacement curve are shown in that order in Figures 4 (a-f). It can be seen that the entangled dislocation structure initially formed at point 2 does not substantially change till point 3 (indentation depth 9.1 Å). During that period, the load increases from 96.2 eV/Å to 198.1 eV/Å, which corresponds to a considerable strain-hardening of the bilayer. This hardening can be attributed to the presence of the interface. In fact, in order to verify the effect of the interface we have also performed indentation of a pure Ni specimen of the same size as the whole bi-layer considered here and observed uninhibited dislocation propagation through the whole layer thickness well before the indentation depth of 9.1 Å. In that case the dislocation structure was also qualitatively different from the one shown in Figs. 3b and 4a.

After a considerable force increase due to the strengthening effect of interface between points 2 and 3, a dramatic force drop is observed between points 3 and 4 on the load-
displacement curve (Fig. 2). At that moment, dislocations finally break through the interface from Ni into Cu. The atomistic configuration corresponding to point 4 is shown in Fig. 4d. Figures 4b and 4c correspond to points 3a and 3b on the load displacement curve and show two intermediate configurations during the fast transition between points 3 and 4. They capture an interesting mechanism. Thus, partial dislocations that initiated in Ni have formed relatively narrow stacking faults (Fig. 3b). However, after they propagated through the interface they widened in Cu (marked with arrow in Fig. 3c). Trailing partial has propagated through both layers and resulted in the step at the bottom. However, the part of the widened stacking fault remained in Cu and started growing back into Ni. This process may be explained by the fact that stacking fault energy (SFE) in Ni is approximately twice higher than that in Cu (see, e.g., Dieter, 1986). It is known that high-SFE metals tend to form entangled dislocations substructures and narrow stacking faults while low-SFE metals have banded arrays of dislocations and wide stacking faults. After the deformation continues between points 4 and 5 the material undergoes another hardening stage. It can be seen that the previously formed stacking fault in Cu layer (marked with arrow in Fig. 4e) seeks to grow back from Cu into Ni, but is stopped at the interface. Finally, at point 6 the partial dislocation breaks through from Cu into Ni and reaches the top surface (Fig. 4f). This type of mechanism has not been observed in the previous study (Medyanik and Shao, 2008) when propagation of dislocations that initiate in Cu and propagate into Ni was investigated.

3.4 Details of dislocation-interface interaction
One interesting phenomenon observed during indentation of the Ni-Cu bilayer is that at certain stage horizontal stacking faults formed at the interface (see Fig. 5). The stacking faults formed either right at the interface between Ni and Cu layers, or in Cu but immediately adjacent to the interface.

The initiation of the horizontal stacking faults is described in Fig. 6. Figures 6a and 6b show the atomic configuration at two successive loading steps at the indentation depth near 9 Å. Here, atoms in perfect lattice are shown in dark blue and Cu-Ni interface is represented by the dashed lines. It is shown that one of the stacking faults (marked as ‘1’ in Fig. 6a) which is bounded by two gliding partial dislocations is transforming into a horizontal stacking fault (marked ‘2’ in Fig. 6b). The mechanism of this transformation is shown schematically in Figs. 6c and 6d. Here, a dislocation core dissociated into leading and trailing partial dislocations is shown interacting with the interface. First, a leading partial is stuck at the interface followed by a trailing partial propagating on the same plane. As the loading continues, the distance between the partials reduces as they are both pressed against the interface. However, instead of further propagating along the initial slip plane, shear of the interface occurs that results in the change of the slip system and the interfacial stacking fault formation.

3.5 Conclusion

Nanoindentation of a Ni-Cu bilayer with coherent (111) interface has been modeled using molecular mechanics simulation. Even though dislocations do propagate through the bilayer, the interface acts as a strong barrier to dislocation propagation and causes a considerable strain-hardening of the bilayer. Dislocation-interface interactions have been investigated and several
specific mechanisms have been observed in the current study. Thus, spreading of a dissociated dislocation core at the interface and interfacial stacking fault formation have been identified and described. Since it is known that stacking faults contribute considerably to materials strain hardening, the mechanism of dislocation-interface interaction that leads to interfacial stacking fault formation can greatly contribute to the overall strengthening of the nanoscale multilayered metallic material.

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References

Fig. 3.1 Initial configuration of a Ni-Cu bilayer with coherent (111) interface.

Fig. 3.2 Load displacement curve for indentation of a Ni-Cu bilayers
Fig. 3.3 Initiation of plastic deformation.
Fig. 3.4 Propagation of dislocation through the interface.
Fig. 3.5 Stacking fault formation at the interface.

Fig. 3.6. Mechanism of a dislocation-interface interaction and interfacial stacking fault formation.
CHAPTER FOUR: INTERACTION OF DISLOCATIONS WITH INCOHERENT INTERFACES IN NANOSCALE FCC-BCC METALLIC BILAYER

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Abstract

Dislocation nucleation and propagation in a Cu-Nb bilayer with an incoherent fcc-bcc interface are examined using atomistic simulations. The nanoindentation model is applied to generate dislocations at and near the surface in one of the layers and push them through the interface into the other layer. The reasons for high strength levels in multilayered metallic composites with incoherent interfaces are investigated. The interface acts as a very strong barrier to dislocation propagation. It is found that even under severe deformation at large indentation depths, no dislocations are transmitted across the interface from Cu into Nb. While dislocation transmission from Nb to Cu can be, in general, observed, it occurs under high loading forces. In both cases, the presence of the interface results in considerable strengthening of the bilayer. Mechanisms of interactions between gliding dislocations and the incoherent interface have been studied in detail. In particular, interface shear at the interface under complex three-dimensional loading conditions are analyzed.
Micro and nano scale multilayered composites often posses unique mechanical properties, such as ultra-high strength levels [1–3]. For example, the strength of metallic nanoscale multilayers can be significantly higher than the strength of bulk materials composing the structure and may approach one half of estimated theoretical strength [3,4]. This remarkable increase in strength is usually attributed to the presence of interfaces that act as barriers to propagating dislocations and cause strain hardening of the multilayered material [5–9].

Mechanical properties of nanocrystalline materials, including nanoscale metallic multilayers, strongly depend on the involved micro-structural length scale, such as the grain size or thickness of the individual layers in the multilayered structure. When layer thickness is on the order of several tens to several hundreds of nanometers, a Hall-Petch effect [11,12] is considered
to be the main reason for the material’s strength increase. According to Hall-Petch relation, yield strength is proportional to the inverse of a square root of the layer thickness $h$:

$$\sigma_y = \sigma_0 + \frac{k}{\sqrt{h}} \quad (1)$$

However, at thinner layers, strength does not obey the Hall-Petch relation anymore. Hall-Petch model, which is based on dislocation pile-up mechanisms, breaks down when individual layer thickness in multilayered systems drops below several tens of nanometers. Creating dislocation pile-ups in such thin layers becomes impossible and essentially new mechanisms that are based on interactions of single dislocations and interfaces start to play major role in strengthening of the nanoscale multilayered metallic materials. According to experimental observations, strength of nanoscale metallic multilayers continues to increase with decreasing individual layer thickness until it reaches a plateau at thickness values on the order of just a few nanometers. The increase in strength strongly depends on the types of metals that compose the multilayered structure as well as on the types of interfaces that form between the layers.

Interfaces in multilayered metallic composites may be generally classified into the following three major categories:

- **Coherent** interfaces form when the two metals at the interface have the same type of lattice structure, e.g., both face-centered cubic (FCC), and the difference in the lattice parameter is relatively small (not more than a few percent).

- **Semi-coherent** interfaces occur when the two metals at the interface have the same lattice type, but the mismatch in the lattice parameter is larger. In this case, networks of misfit dislocations form at the interface to accommodate the mismatch.
• Incoherent interfaces form between materials with different lattice structures, such as, e.g., FCC and BCC (body-centered cubic).

It should be noted that both coherent and semi-coherent interfaces may form in multilayers that consist of metals with the same lattice structure and a small mismatch in lattice parameter. In that case, the occurrence of a particular type of interface depends on the individual layer thickness. For relatively thin layers, fully coherent interfaces are more favored energetically; however a loss of coherency usually occurs when layer thickness exceeds some critical value [10].

Mechanisms of dislocation-interface interactions that dominate plastic deformation of metallic multilayers with thin layers are strongly dependent on the type of interface. Thus, in the case of coherent and semi-coherent interfaces when both materials have the same crystal structure, slip planes and directions are nearly continuous across the interface. For this reason, such interfaces are also called transparent. In this case, a mismatch at the interface in such properties as lattice constant, elastic modulus, and dislocation core energy dominate the dislocation-interface interactions. Thus, e.g., mismatch in lattice constant leads to coherency stresses near the interface that strongly influence propagation of dislocations. Furthermore, in multilayers with semi-coherent interfaces, pre-existing networks of misfit dislocations often dominate plasticity. In the case of incoherent interfaces when crystal structures of the two materials are different, the slip planes and directions are discontinuous across the interface. Such interfaces are also sometimes called opaque. In this case, the crystallographic discontinuity of slip systems becomes a major factor that may inhibit a slip transmission across the interface. Apparently, the case of each interface, and possibly even each pair of metals comprising the interface, is quite unique and has to be separately addressed; deriving a general type of formula,
similar to Hall-Petch model’s equation (1) to describe strengthening of multilayered materials with very thin layers seems hardly possible in this case.

A number of researchers have employed atomistic simulations using empirical interatomic potentials to study the nucleation and propagation of dislocations in materials with grain boundaries and interfaces [13-19]. However, most of these studies focused on interfaces and grain boundaries in bi-crystals comprised of the same material. Very rarely have interfaces between dissimilar materials been considered and even in that work most effort has been focused on coherent and semi-coherent interfaces. Relatively small amount of work has been published that addressed the issues of incoherent interfaces in nanoscale metallic multilayers. Hoagland and co-workers have studied incoherent Cu-Nb interface [7,20]. That work was focused on the interaction of single, artificially introduced dislocations with the interface under essentially two-dimensional modeling conditions. More recently, Wang et al. [21] used a similar approach to examine in more detail the influence of the interface structure on dislocation-interface interaction. Under a compressive load normal to the interface or a tensile load parallel to the interface, three types of interfaces and three types of full dislocations were considered. All that work has provided valuable insights into the mechanisms of interaction between dislocations and incoherent interfaces. However, it would be interesting to investigate how these (and perhaps other) mechanisms may work in a different simulation set-up, under essentially three-dimensional loading conditions, such as nanoindentation, when dislocations repeatedly nucleate, move, and interact with incoherent interface. To the authors’ knowledge, no such studies have been performed to date.
Nanoindentation is often employed to study mechanical properties of materials in both experiments and simulations. In simulations, nanoindentation is especially convenient as it allows for consistent generation of dislocations under the indenter and observation of their subsequent propagation into the domain. A number of researchers have modeled nanoindentation using atomistic simulations in order to study dislocation nucleation and propagation in metals [22–27]. However, in most cases, *homogeneous* dislocation nucleation in perfect single crystals has been considered when dislocations nucleate beneath the indenter at a point where maximum resolved shear stress reaches a critical value needed to initiate a slip for a given slip system. However, when the material’s atomic-scale structure becomes more complicated due to the presence of various defects, such as pre-existing dislocations, impurities, vacancies, grain boundaries and interfaces, *inhomogeneous* dislocation nucleation occurs in a much more complex manner. For details on recent progress in the area of nanoindentation, both modeling and experimental, the reader may refer to the recent review articles [28,29].

In this work, we perform atomistic simulation studies of nanoindentation into a Cu-Nb bilayer with an incoherent interface and focus on the effects of the interface on dislocation propagation. The nanoindentation model seems to be especially convenient as it allows for generation of dislocations at and near the surface and observation of their propagation into the bilayer’s volume. We apply indentation from each of the Cu and Nb sides of the bi-layer in separate simulations. This approach helps to investigate the mechanisms of dislocation -interaction in both metals. It also assists to explore the overall hardening behavior and strengthening effects of the interface and analyze the influence on these two properties imposed by the stacking sequence of the metals based on the obtained load-displacement relations.
4.2 Computational methodology

4.2.1. Embedded-atom method potential

In this work, molecular mechanics simulations are performed utilizing the embedded-atom method (EAM) [30,31] to model interatomic interactions. In the EAM, each atom in a material is treated as an impurity embedded in a host containing all other atoms in the material. This method is capable of dealing with various kinds of metallic systems which can include such features as fractures, surfaces, impurities and alloying addition. The total energy of a system of atoms is given as

\[ E_{\text{tot}} = \sum_i F_i (\rho_i) + \frac{1}{2} \sum_{i \neq j} \phi_{ij} (R_{ij}) \] (2)

where \( F_i \) is the embedding energy which is a function of the atomic electron density \( \rho_i \) at atom site \( i \), \( \phi_{ij} \) is a pair potential interaction, and \( R_{ij} \) is a distance between atoms \( i \) and \( j \). The particular form of the EAM potential used in this work is of the type given by Voter and Chen [32,33], Johnson and Oh [34] and Hoagland et al [7] for describing the interaction of Cu-Cu, Nb-Nb and Cu-Nb, respectively. These potentials was derived to fit several parameters obtained from experiments (lattice and elastic constants, cohesive and vacancy formation energy, energy of mixing, etc) and ab-initio simulations, and has been shown to provide good approximations in terms of generalized stacking fault energy [35], lattice stability [7,34] and behavior of Cu-Nb interfaces [7,20,21,36,37]. The molecular mechanics simulations employ the conjugate gradient
procedure for energy minimization and are performed using the parallel atomistic simulation
code LAMMPS developed at Sandia National Lab [38,39].

4.2.2. Visualization of defects

In order to study lattice defects in general and dislocation nucleation and propagation in
particular, we need to reliably locate those defects within the crystal structure. Several different
approaches have been commonly used for this purpose based on different criteria, such as,
atomic excess energy or coordination number. Kelchner et al. [22] introduced another way of
visualizing defects in crystals: centro-symmetry parameter. In a perfect centro-symmetric crystal
(i.e., FCC or BCC), each atom has a given number of nearest neighbors (twelve for FCC, eight
for BCC). Based on this, the centro-symmetry parameter for a given atom is defined as follows:

\[ P = \sum_{i=1,\alpha} |\mathbf{R}_i + \mathbf{R}_{i+\alpha}|^2 \]  

(3)

where \( \alpha \) is the number of the pairs of nearest neighbors, i.e. for BCC \( \alpha \) is 4 and for FCC \( \alpha \) is 6, \( \mathbf{R}_i \)
and \( \mathbf{R}_{i+\alpha} \) are the vectors that corresponds to the pairs of the opposite nearest neighbors. A centro-
symmetric material, such as FCC or BCC metal, tends to preserve its centro-symmetry under
homogeneous elastic deformation. Thus, if the material deformation is nearly homogeneous, the
value of \( P \) is close to zero. However, if the material has defects present where its centro-
symmetry is destroyed, \( P \) will no longer be zero for the atoms comprising the defects. Instead,
the parameter will have a value within the range that corresponds to a particular defect. Thus, for
Cu (FCC), values of the centro-symmetry parameter for atoms comprising partial dislocation
loops and stacking faults are about 1.6 Å$^2$ and 6.4 Å$^2$ respectively; for Nb (BCC), because there is no stacking fault or partial dislocation, the centro-symmetry parameter value for atoms comprising dislocation loops is about 4.1 Å$^2$.

In this work, we use a functionality of AtomEye [40] to compute the centro-symmetry factor $c$ (although using the same basis, AtomEye gives different values of centro-symmetry parameter. To distinguish, we call this value as centro-symmetry factor). Following the same basis as Kelchner’s approach, AtomEye performs the calculation in a slightly different way. The centro-symmetry factor of an atom is given as

$$
c = \frac{\sum_{i=1}^{\alpha}|R_i + R_{i+\alpha}|^2}{2\sum_{j=1}^{2\alpha}|R_j|^2}\tag{4}
$$

where $\alpha$, $R_i$, and $R_{i+\alpha}$ have the same meaning as above, $R_j$ stands for the each vector that corresponds to the pair of nearest neighbors. The difference between $c$ and $P$ is that $c$ is normalized as a dimensionless quantity and varies from 0 to 1. The centro-symmetry factor values for FCC materials are 0.01 and 0.04 for atoms comprising partial dislocation loops and stacking faults, respectively. For dislocation loops in BCC material, the centro-symmetry factor is 0.03.

4.3 Results

In this work, two simulations of nanoindentation are carried out on different sides of two identical atomistic configurations of a Cu-Nb bi-layer. When the indenter is applied to the Cu side of the bi-layer, the simulation is denoted as Cu-Nb; and the case when the indenter is
applied to the Nb side is denoted as Nb-Cu. In this section, the initial configuration of the bi-layer is first introduced and the interface between Cu and Nb is closely examined. Then, the obtained force-displacement curves of the simulations are presented and analyzed with references to the snapshots of the atomistic configurations. The interaction of dislocations with the interface in both Cu and Nb is studied. Finally, the results of the two cases of indentation are compared to each other and to some other results available in the literature.

4.3.1 Initial configuration and bi-layer interface

The simulation setup is shown in Figure 1. Two slabs of metals are placed one on top of another. Following the Kurdjumov-Sachs epitaxial orientation such that \( \{111\}_{\text{FCC}} \parallel \{110\}_{\text{BCC}}, \) \( <110>_{\text{FCC}} \parallel <111>_{\text{BCC}}. \) The dimensions of the computational cell are 172 x 60 x 172 Å; each layer has a thickness of 30 Å. According to the experimental data \[20\], at this individual layer thickness the structure should demonstrate a peak strength. The interface between the two materials is parallel to \( x-z \) plane. Lateral sides (faces perpendicular to the \( x \) and \( z \) directions) of the bi-layer are fixed, while free boundary conditions are applied at the top and bottom surfaces. The boundary conditions of this particular model are chosen to fully isolate the interaction of the dislocations with the interface, i.e. the propagation of dislocations will not be interfered (say, by a fixed bottom). A nearly rigid spherical indenter with radius \( R = 40 \) Å, modeled using quadratic repulsive force, is applied to the center of the top surface. At each step, the indenter is lowered by 0.1 Å and equilibrium configuration is found using energy minimization. The steps are repeated until the total indentation depth has reached 20 Å. It is important to note that in the experimental works of nano-indentation the radii of the indenter tips as well as the indentation depth are commonly much larger than the current simulation, whereas the individual layer
thicknesses of the multilayers are comparable to this work. This indicates that, in reality, much more layers are affected by the stress imposed by the indentation. To account for this, the indenter radius of 40 Å was chosen in this work, which will make the stress deep enough to affect the interface. Meanwhile, the aspect ratio of the computation cell is chosen to make sure that the dislocations can propagate to the bottom (if they eventually can) before they are interfered by the rigid walls (fixed boundary conditions on the sides).

One noticeable feature of the initial configuration is that two sets of slip planes, one set in Cu and one set in Nb, share a common intersection line with the interface plane, although there is a small angle of 10.5º between them. Figure 2 shows these slip planes from a side view. The dashed lines represent one pair of slip planes in Cu (white) and Nb (black). In this case, the resolved shear stress in one plane will maintain most of its value into the other plane. Hence, they are the favored planes for cross-interface transmission of dislocations. Note that it is impossible for the same dislocation to propagate through the interface between Cu and Nb, because Cu and Nb have different lattice types dislocation Burger’s vectors differ in these two materials. However, due to the stresses imposed at the interface by the dislocation in one layer, a new dislocation may nucleate and propagate in the other layer. This process is called dislocation transmission.

During relaxation of the initial configuration, atoms near the interface rearrange seeking their equilibrium positions. The Cu and Nb sides of the interface are shown in Figure 3. Atoms here are colored according to their excess potential energy (relative to the potential energy of atoms in a perfect bulk material). Similar to the results observed by Hoagland et al. [7], a periodic unit cell (indicated by white parallelograms in Figure 3) is found in the Cu-Nb interface. The corresponding atomic displacement field is plotted in Figure 4. The vectors represent
displacements of the relaxed interface on both Cu (left) and Nb (right) sides relative to the unrelaxed configuration. An array of repeating circular regions with atoms moving in a vortical manner can be found on both Cu and Nb sides of the interface. A similar vortical structure at the Cu-Nb interface has been observed in [7]. It can also be seen that the displacements of atoms on the Cu side is much larger than those on the Nb side.

4.3.2. Indentation on Cu-Nb bi-layer

First, we perform indentation of the bilayer from the Cu side as shown in Figure 1. Figure 5 demonstrates the load displacement curve for indentation of a Cu-Nb bi-layer. A noticeable phenomenon of the Cu-Nb indentation is that the material hardens significantly after the yield point. During the indentation process, there are no major drops of load and the load grows fairly steadily throughout the indentation. Snapshots of the atomistic configurations corresponding to points marked on the load-displacement curve are shown in Figure 6. As can be seen in Figure 5, yielding occurs after the depth of 5.8 Å (point 1). Figure 6a shows the atomistic configuration corresponding to point 1. At point 2, a few dislocations nucleate, and a load drop is observed. A snapshot of the atomistic configuration that corresponds to point 2 is shown in Figure 6b. All dislocations nucleated at point 2 are confined in the Cu layer, and there are no dislocations nucleated in the Nb layer. From point 2 to point 5 (Figures 6b to 6e), the load continues to grow with some minor fluctuations which are due to the nucleation of new dislocations in Cu. The transition of one of these minor force drops (between points 3 and 4) is shown in Figures 6c and 6d.

As can be seen from Figures 6a-6d, many dislocations formed beneath the indenter; however, dislocations still cannot penetrate the Cu-Nb interface. At point 5 and point 6, a rather
complex network of partial and full dislocations form, and Nb layer has deformed quite significantly, but no dislocations can be transmitted to the Nb layer. The load drop between points 5 and 6 is due to the nucleation of several new dislocations in Cu.

From Figure 6, one can see that although large numbers of dislocations propagate through the Cu layer, there are no dislocations transmitting across the Cu-Nb interface. This makes the behavior of dislocations worth paying special attention to when they reach the Cu-Nb interface. Hoagland et al. pointed out that interfaces in single and multiphase polycrystalline materials can absorb or trap lattice dislocations [7]. When the dislocations reach the Cu-Nb interface, the core of the dislocations spreads within the interface causing the interfacial shear.

Figure 7 shows the interface displacement fields on the Cu and Nb sides when dislocations reach the interface (at indentation depth of 5.9 Å, point 2 in Figure 5). The point at which dislocation junctions meet the interface is marked using red (solid) lines. It is apparent that when dislocations interact with the interface, the displacement magnitudes on the Cu side are much larger than those on the Nb side. Hence, interfacial shearing must have happened. Closer inspection reveals that inside the area marked by red (solid) lines, the material on the Cu side of interface is flowing outward; a similar trend is observed at the Nb side of the interface but to a much smaller degree. The material flow of this process is depicted schematically in Figure 8. At the onset of the dislocation-interface interaction, the bulk material flows down along the two slip planes, $(1\bar{1}1)$ and $(\bar{1}11)$, marked in Figure 8, while the material close to interface is moving laterally. Both directions of flows are marked using arrows.
4.3.3. Indentation of Nb-Cu bi-layer

Now, the bi-layer is indented from the Nb side. The load displacement curve is plotted in Figure 9. In contrast to previous case where the indenter is applied on the Cu side, this curve is even smoother. Snapshots of the configuration that corresponds to the numbered points marked with arrows are given in Figure 10. When indented from the Nb side, the bi-layer yields at point 1 in Figure 9; at this point dislocations have nucleated in the Nb layer (Figure 10a). As the loading continues, more dislocations nucleate, propagate and are finally trapped at the interface (Figure 10b). At point 3 in Figure 9, so many dislocations have been trapped at the interface in the Nb layer that the resulting concentration of stress in the Cu side of interface is high enough for dislocations to nucleate. Figure 10c shows the nucleation of the first dislocation (marked with an arrow) in Cu. At point 4 in Figure 9, more dislocations in Nb have been arrested at the interface, which provides sufficient stress for dislocations to propagate through the Cu layer. From Figure 10d, one can see that the dislocation in Cu has expanded and propagated to the bottom. A full surface step can be seen forming on the bottom (marked with a black arrow). Followed by that, at point 5, there is a little drop of the indentation load. Comparing Figure 10d to Figure 10e, one can see that there is no significant change in the structure of the dislocations in Cu; hence, the load drop is mainly due to the formation or propagation of the dislocations in Nb. As the load continually climbs throughout the whole indentation process, the maximum load (about 240 eV/Å) is reached at point 6 on the load-displacement curve.

Similar to the case in the previous section, due to the “weak” nature of the Cu-Nb interface, the dislocation cores spread when they come into the interface and a quite noticeable interfacial shear takes place in the Nb-Cu bi-layer. Figure 11 shows the vector fields of the Cu and Nb sides of the interface while the first dislocation in Cu is nucleating. It can be seen that
even for a very small portion of the loading stage, interfacial shearing is occurring quite commonly. The red line represents the trace where the slip plane of the dislocation intersects the interface. Here, although the interface tries to absorb the dislocations from Nb, due to the relatively large Burger’s vectors of Nb dislocations, the interface cannot accommodate them as efficiently as it does for the Shockley partials in Cu. Hence, the Nb dislocations form ledges on the interface and nucleate dislocations in Cu.

It is important to note that unlike the case considered in the previous section, in the simulation of indentation on Nb-Cu, dislocations do transmit through the Nb-Cu interface. Furthermore, in Section 3.1, one pair of slip planes in Cu and Nb, $(11\overline{1})_{\text{Cu}}$ and $(01\overline{1})_{\text{Nb}}$, have been identified as such that dislocation transmission is likely to occur on these planes. However, instead of transmitting between these planes, the dislocations transmit from a $(0\overline{1}\overline{1})_{\text{Nb}}$ plane to a $(\overline{1}1\overline{1})_{\text{Cu}}$ plane. The intersection lines of these slip planes with the interface have an angle of $10.5^\circ$. The spatial configurations of the two slip planes are depicted in Figure 12.

Figure 13 shows the transmission of the dislocations from a side view of the cross section of the domain. The dislocation shown in the figure has propagated through the Nb layer and stopped at the interface causing a Shockley partial to nucleate and propagate through the Cu layer. In Figure 13b, the leading partial in Cu has reached the bottom leaving a stacking fault in the $(\overline{1}1\overline{1})_{\text{Cu}}$ plane (solid line). The Burger’s vector of the dislocation in the Nb layer has been identified as $b = \alpha \cdot \frac{a}{2}[111]$, where $\alpha$ is a fraction of 1, because this is clearly not a full dislocation. In Nb, there are so many slip systems available, that several slip systems tend to be activated at the same time and the dislocations tend to entangle with each other. This, together with the fact
that the layer thickness is small, makes it hard to clearly define a full dislocation. The Burger’s vectors for the leading partial in the Cu layer is $b = \frac{a}{6}$ \[121\].

Dislocation transmission between Cu and Nb has been observed by other researchers in the past few years. For example, Hoagland et al. studied the interaction of a dissociated glide dislocation in Cu with the Cu-Nb interface \[20\]. In that work, a dissociated dislocation was placed in Cu, and a uniaxial tensile strain was applied to the bi-layer. As a result, the original dislocation entered the interface, and two new glide dislocations have emerged in Cu and Nb, respectively. In other words, a dislocation has been transmitted from Cu to Nb. This seems contradictory with the findings in this work. However, a closer look at the applied stress in the two works can reconcile the contradiction. In Hoagland’s work, at the stage when the transmission was happening, the applied uniaxial strain was about 3.5% in both layers. This strain produces very high tensile stresses about 7 GPa in Cu and 4.5 GPa in the Cu and Nb layers. The maximum resolved shear stress in their slip planes are about 2.2 GPa and 2.0 GPa in Cu and Nb respectively. In our study, the loading conditions and the dislocations from Cu at the end of the indentation process make the stress distribution highly inhomogeneous. However, by examining the regions close to the interface in Nb layer, we can safely tell that our resolved shear stress level is about 1 GPa, which is significantly smaller that Hoagland’s work. Hence, it makes sense that they eventually observed the transmission, and we, being more realistic, do not.

Wang et al. tested the interaction of three types of dislocations and three types of Cu-Nb interfaces \[21\]. In their work, dislocations were first placed in the model (either in Cu or in Nb), and then uniaxial tension or compression was applied. It turned out that even with large stresses applied, dislocation transmission from Cu to Nb did not happen. While at a certain stress level, a
mixed dislocation initially in Nb was reported emitting a Shockley partial in Cu near the interface. However, in these cases the slip planes in which the transmission occurred share the same trace of intersection on the interface, although they are misoriented by a small angle. This is different from what is observed in this work.

4.4 Conclusion and Discussion

We have performed molecular mechanics (MM) simulations of nanoindentation on Cu-Nb bi-layers with different stacking sequences. Differences between the two Cu-Nb models can be found if we inspect their curves carefully. First, they demonstrate two different levels of stiffness for the same Cu-Nb bi-layer if indentation is applied on different metallic materials. Cu has a higher Young’s modulus than Nb. Hence, if applied on Cu side, the indenter encounters a stiffer response than on the Nb side. Second, the yield load is higher if the indenter is applied to the Nb side. This makes sense because unlike Cu, Nb is a body centered cubic (BCC) metal and none of its slip systems are close packed. Hence, it is very difficult to activate the slip systems in Nb unless a sufficiently large resolved shear stress is applied. Finally, in the plastic regime, Nb-Cu hardens at a faster rate than Cu-Nb and in a fashion without significant load drops. This is because, as a BCC metal, Nb has 48 slip systems that are nearly close packed. There are always several slip systems that are oriented so that they are ready to slip. Quite commonly, dislocations nucleated in one slip plane may interfere with dislocations in other slip planes, and thus lead to a strengthening of Nb.

The interaction of dislocations with Cu-Nb interfaces has been studied previously by several other researchers via atomistic simulation methods [7,20,21]. However, in their works, a dislocation was always placed in the computational cell which is subject to either a
uniaxial/biaxial load or no load. Dislocation transmission was observed in some of the works; in those works, the involved slip planes share a common intersection line in the interface. In this work, instead of “planting” dislocations in the model, we have multiple dislocations naturally generated in three dimensional indentation. Prior to the indentation, the initial configuration was relaxed and an interfacial rearrangement is observed. This agrees with what has been found in the previous work [7]. During indentation, it can be seen that the Cu-Nb interface is absorbing dislocations and acting as a major barrier to dislocation transmission. When dislocations reach the interface from the Cu side, a pattern of material flow as well as interfacial shear is observed. No dislocations can be seen transmitting from Cu to Nb when the indenter is applied to the Cu side of the bi-layer, even at a very deep indentation depth. However, when indenting from Nb side, although considerable amount of interfacial shear occurs, transmission of dislocations does happen from Nb to Cu. The transmission occurs between a pair of slip planes such that their intersection lines with the interface have an angle of 10.5º (see Figure 11).

It is also interesting to note that the interaction of dislocation and interfaces due to the low shear strength of the Cu-Nb interface observed in this work could be generally valid for all FCC-BCC interfaces that follow the KS (Kurdjumov-Sachs) relations. As pointed by Wang et al [36], the shear strength of a Cu-Nb interface not only depends on the interaction between the Cu and Nb atoms, but also on the atomic arrangement of the interface. The low shear strength feature of a KS Cu-Nb interface seems to be general feature for all KS oriented FCC-BCC interfaces.

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Figure 4.1 Initial configuration for a Cu-Nb bilayer shown with indenter applied to the Cu layer. Top layer (light brown) is copper, bottom layer (gray) is niobium. The interface is FCC (111) plane for copper, and BCC (110) plane for niobium. The indenter radius is $R = 40 \, \text{Å}$.

Figure 4.2 Side view of the slip planes in Cu and Nb, which have a common intersection line at the interface.
Figure 4.3 Atomic planes at the Cu-Nb interface. The bi-layer configuration is cut into two parts along the interface. The atoms are colored according to their excess potential energy.

Figure 4.4 Vector fields visualizing displacements of atoms at the interface on Cu (left) and Nb (right) sides after relaxation. Displacements are taken in reference to the initial configuration that has not been relaxed. Vectors are colored according to their magnitudes of net planar (x-z plane) displacement.
Figure 4.5 Load displacement curve of Cu-Nb.
Figure 4.6 Snapshots of the atomistic configuration of Cu-Nb at different stages of indentation. Here, two metallic layers of atoms are shown separately. The top layer is Cu and the bottom layer is Nb. Atoms are colored according to their centro-symmetry parameter values and are not shown if they are in perfect FCC lattices.
Figure 4.7 Vector fields of atomic displacements for the Cu (left) and Nb (right) sides of the interface after the first dislocation reaches the interface. Displacements are measured relative to the positions of atoms in the relaxed configuration before applying indentation.
Figure 4.8 A schematic representation of the material flow due to interface shearing when dislocations reach the Cu-Nb interface.

Figure 4.9 Load displacement curve of Nb-Cu.
Figure 4.10 Snapshots of atomistic configuration of Nb-Cu at different stages of indentation. Atoms are shown following the manner of Figure 6.
Figure 4.11 Vector fields of atomic displacements for the Cu (left) and Nb (right) sides of the interface when the first dislocation in Cu nucleates.

Figure 4.12 Schematic depiction of the slip plane on which dislocation transmission occurred.
Figure 4.13 Transmission of dislocation from Nb into Cu. The computational domain is cut along the yellow (solid) line in (a), (b) is a view along the white (dashed) arrow in (a). In (b), the dashed line represents $(0\bar{1}1)_\text{Nb}$ plane in Nb, while the solid line represents $(\overline{1}1\overline{1})_\text{Cu}$.

Figure 4.14 Load displacement curve for Cu-Nb, Nb-Cu
CHAPTER FIVE: EFFECT OF INTERFACES IN THE WORK HARDENING OF NANOSCALE MULTILAYERED METALLIC COMPOSITES DURING Nanoindentation: A MOLECULAR DYNAMICS INVESTIGATION

S. Shao, H. M. Zbib, I. Mastorakos, and D.F. Bahr

Abstract

The strain hardening and the related surface pile-up effect of the CuNi, CuNb and CuNiNb multilayers are considered using atomistic simulations of nanoindentation on such multilayers with varying individual layer thickness. Using empirical load-stress and displacement-strain relations, the obtained load-depth curves were converted to hardness-strain curves which was then fitted using power law. It is found that the extent of surface pile-up is inversely related to the hardening exponent of the NMMs. After examining the deformations on and below the top surfaces, two mechanisms of the surface pile up are discovered and discussed. The first mechanism involves the propagation of dislocations intersecting the top surface, and is sensitive to the Burger’s vector. The second mechanism is governed by a special Lomer-Cottrell-type dislocation reaction. From the stress-strain data, it is discovered that interfaces and their type play a major role in hardness; hardness increases with strain when incoherent interfaces are present. The hardening parameters are found to be functions of the interfacial dislocation density, which in turn is power law dependent on two length scales: indentation depth and individual
layer thickness. A constitutive model describing strain hardening in NMM under nanoindentation is developed.
5.1 Introduction

In the recent years, a new family of composite materials, namely Nanoscale multilayer metallic (NMM) composites are developed and have attracted significant amount of attention among the materials research communities. This type of material, when the individual layer thickness is within several nano meters, can achieve exceptional strength levels [1-3]. The high strength of these composites can generally be attributed to the strain hardening caused by the presence of interfaces which impede the free propagation of dislocations [4-8]. When the individual layer thickness is above 50 nm, dislocation pile-up at the interfaces is the controlling mechanism. The stress at the tip of the pile-up is significantly higher than that produced by a single dislocation. With this mechanical advantage, the slip is relatively easy to continue to the next layer (slip transmission). The strength of the composite obeys the Hall-Petch relation. When the individual layer thickness drops lower than 50 nm to several nanometers, the room for dislocation pile-up is limited and afore mentioned mechanical advantage is then gradually removed. Thus, the strengths of NMM composite at this thickness range are considerably higher. Also, the controlling mechanism becomes the interaction between single dislocations with interfaces (e.g. confined layer slip-CLS, single dislocation transmission, etc); hence the Hall-Petch relation breaks down. The interaction of dislocation with different types of metallic interfaces has been a very hot topic and has been reported in quite a few works [4-15]. Among which models are proposed to predict the strength of composites with particular types of interfaces. For instance, Hoagland et al [8] has refined the CLS model based on the experiment data of hardness of Cu-Nb multilayer and proposed a new model that takes the interface stress and the interaction between the threading dislocations and the pre-existing interfacial dislocations into account. Akasheh et al [12] have investigated the CLS in Cu-Ni multilayers with pre-existing interfacial
dislocations and suggested that the barrier exerted by such dislocations to the new threading dislocation is critical to the strength of the material. Based on such suggestion a model was proposed. Currently, a good amount of experimental studies using nanoindentation to explore the strain hardening of NMM composites are available [16-18]. However, there are only very limited theoretical and numerical studies that address the strain hardening of NMM composites and how it relates to nanoindentation and the underlying material structure, i.e. individual layer thickness and types of the interface (coherent or incoherent). A recent work by Bellou et al [17] considered Cu-Ni-Nb- based bilayer and trilayer systems and showed that the CuNiNb trilayer system displays higher strain hardening rate than either CuNi or CuNb bilayer systems. In that work, various loading techniques have been employed to reach different effective strain levels, including bulge testing and nanoindentations using Berkovich and cube corner tips. Interestingly, this partially agrees with the findings of the current paper. However, the experiments in that work only examined a series of CuNi, CuNb and CuNiNb NMMs with individual layer thickness of 20 nm. Therefore, in the current work, using molecular dynamics and mechanics, the deformation of NMM composites with different underlying structures (composition, individual layer thickness, etc) under spherical nanoindentation conditions is addressed.

In the past few decades, indentation has been widely used to probe materials mechanical properties, such as hardness, elastic modulus, etc. for its unique features such as simplicity, cost effectiveness (can perform multiple indentations on a single sample), non-destructiveness, low requirement for specimen preparation, wide range of applications (bulk, thin films, nanostructures, and even biomaterials) etc [19]. Nowadays, with the advance of technologies, the sensitivities of the load and displacement in the commercial indentation systems have been decreased down to the level of pico-newtons and nanometers. Thus, a new class of indentation
techniques – nanoindentation - has emerged. The nano-indentation is most commonly used to test the nanosized material systems, e.g. thin films, micro-pillars, carbon nanotube forests, thin biofilms, etc. Nanoindentation essentially introduces a three dimensional stress state to the materials being tested, which is a relatively more realistic loading condition, hence it is also adopted quite commonly in atomistic studies. For instance, quite a few of them have investigated the interaction between interfaces and dislocations using nanoindentation as a dislocation generator. Van Vliet et al. [20], Ju et al. [21] and Hasnaoui et al.[22] performed nanoindentations on Cu, Al, Ni and Au. These studies focused on the interfaces in bi-crystals and grain boundaries in nanocrystalline materials. Such materials are comprised of the single metals; no interfaces between dissimilar metals have been considered. Recently, Saraev and Miller have studied copper multilayers [23] subjected to nanoindentation using atomistic simulations where different numbers of $\Sigma$29 twist grain boundaries were considered. Copper single crystal nanometer-sized nickel coatings [24] were also considered in the same context. In this work, the semi-coherent Cu-Ni {111} interfaces separating the Ni coating and Cu substrate were considered. It was found that the mechanics of plastic deformation of the composite during nanoindentation was dominated by the misfit dislocation networks and strongly depended on the initial position of the indenter with respect to the misfit dislocations. More recently, Shao and Medyanik [13-15] have investigated the interaction between dislocations and the coherent Cu-Ni and incoherent Cu-Nb interfaces using bilayer models under nanoindentation. It has been found that, both Cu-Ni and Cu-Nb interfaces are responsible for the strain hardening of the NMMs. However, the Cu-Nb interface is a much stronger barrier to propagation/transmission of gliding dislocations compared to Cu-Ni interface. More generally, it was anticipated that the blocking effect of the FCC-BCC incoherent interfaces is stronger than that of the coherent FCC-FCC interfaces.
An interesting issue for nanoindentation needs to be addressed is the surface pile-up/sink-in effect. During a nanoindentation, the material surface around the indented impression can either bulge out or sink in. This can significantly impact the mechanical properties of material measured by this technique. First, the pile-ups and sink-ins can affect the measurement of the contact radius and area which directly affects calculation of the hardness values [25-27]. Second, the height of pile-ups and depth of sink-in have a strong relation to the strain hardening rate of the material being test [28]. The extent of the surface pile-up effect could be an indication on the material’s strain hardening rate. In the experiments of nanoindentations on CuNb, CuNi and CuNiNb multilayers, it has been found that different pile-up heights has been observed for these multilayers, and the ranking of the pile-up heights is inverse to that of the hardening exponent of the multilayers [17]. The surface pile-up effect during indentations has been investigated before by addressing the plastic deformation underneath an indenter using the slip line theory. Indenters with different shapes, e.g. wedges and cones, different boundary conditions, friction and frictionless have been considered [29]. These investigations focused on a macro scale, the materials considered were treated as continuum. To explain the pile-up effect in the NMM composites, the interfaces and their interactions with the dislocations have to be taken into account. However, explanations to the surface pile-up and sink-in effect from such perspectives are still lacking. Atomistic simulations seem to be an effective tool for such task.

Hence, in this work, spherical nanoindentations on metallic nanolaminates are performed using atomistic simulations. The relation between the pile-up extent and the measured hardening exponent of the nanolaminates will be analyzed. The plastic deformation of the multilayers are carefully examined; the mechanisms of the surface pile-up in NMM composites is captured and explained in detail. The strain hardening behavior of the NMM composites is investigated. The
hardening parameters $n^*$ and $K^*$ are related to the interfacial shear deformation and the geometric parameters of the NMMs. A model describing constitutive behavior of NMM composites under nanoindentation is proposed.

5.2 Problem set up

In this work, molecular dynamics (MD) and molecular mechanics (MM) simulations of nanoindentations are performed on Cu-Ni-Nb- based metallic multilayers, i.e. CuNi, CuNb and CuNiNb. Note that the sequence of the elements in such notations denotes the stacking sequence of the NMM composites from top to bottom, e.g. CuNi refers to a Cu-Ni- based multilayer system with a stacking sequence of Cu-Ni-Cu-Ni…. Among all the simulations, various individual layer thicknesses ($h = 2, 3$ and $5$ nm) and indenter radii ($R = 6, 9$ and $15$ nm) are included and all possible combinations of the two are all covered. 27 simulations were performed in total for the three types of NMM composites. As shown in Figure 1, the size of the simulation cell is approximately $400 \times 400 \times 400$ Å$^3$, with periodic boundary conditions applied on the four side faces, fixed on the bottom and free on the top surface. The indenter is applied on the top surface. The crystallographic orientations of the layers with respect to the current coordinate system are as follows: $x//[11\bar{2}]_{\text{CuNi}}//[\bar{1}\bar{1}2]_{\text{Nb}}, y//[111]_{\text{CuNi}}//[\bar{1}\bar{1}0]_{\text{Nb}},$ and $z//[\bar{1}\bar{1}0]_{\text{CuNi}}//[111]_{\text{Nb}}$. The models involve coherent CuNi interfaces (FCC-FCC) and KS1 [9] incoherent CuNb and NiNb interfaces (FCC-BCC). Necessary strains are applied to Cu, Ni and Nb layers to guarantee coherency and registry [30]. The atomistic systems are relaxed using energy minimizations (molecular mechanics) before being indented. The simulations of indentation are performed using molecular dynamics (MD) with indentation speed of $5$ m/s. A MD simulation package
LAMMPS [31-32] is used. Atomic pair interactions among all the elements, i.e. CuNi [33], CuNb [6], NiNb [34], are modeled using EAM potentials. Such potentials have been widely used in the past few years, and have shown good performance dealing with defects, e.g. interfaces and vacancies [5, 9-10, 13-15, 35].

5.3 Results and Analyses of the Atomistic Studies

Load-depth curves were obtained from simulations with different combinations of layer thickness and indenter radii for nanoindentations on CuNb, CuNi and CuNiNb systems. The load-depth curves are shown in Figure 2a. Typical results are chosen and shown in Figure 3a for the three types of multilayers (CuNi, CuNb and CuNiNb) with layer thickness $h=30\AA$, indented by indenters with radius $R=90\AA$. As can be seen, higher the yield load and stiffness for CuNi differs quite noticeably from those of CuNb and CuNiNb: they are both higher. As discussed by Shao and Medyanik [15], the presence of FCC-BCC interface decreases the yield load for CuNb and CuNiNb multilayers and the fact that Cu and Ni has higher Young’s modulus than Nb causes the difference in stiffness.

The obtained load-depth curves are then converted to hardness-strain curves using the following commonly used load-hardness and depth-strain relations: (1) The hardness of a material during an indentation test is defined as the mean pressure below an indenter: $H = P/A$, where $P$ is the load of indentation, and $A$ is the contact area. Similar to what was done in Saraev and Miller’s work [24], the contact area is measured from the number of the atoms in direct contact with the indenter. The contact radius $a$ is then calculated as $a = \sqrt{A/\pi}$. (2) According to Johnson [36], an effective strain can be estimated from the displacement data collected from a
spherical indentation by $\varepsilon = 0.2a/R$, which then can be compared to the data obtained from tensile test. Thus, the plastic regimes of the load-depth curves are converted to hardness-strain curves and shown in Figure 2b. We can fit the plastic hardness-strain response of the multilayers using a power law model of the form:

$$H^* = K^* \varepsilon^n$$

(1)

O’Neil [37-38] and Tabor [39] has shown that for homogenous film the value $n^*$ obtained from the indentations is equivalent to the strain hardening exponent obtained from the tensile test, where a stress-strain curve ($\sigma=\sigma_0 \varepsilon^n$) is measured. Also, there exists a relation between $K^*$ and $\sigma_0$ as was shown in [39]. However, finding this relation is beyond the scope of this work, thus will not be discussed here. The plastic regimes of all 27 converted hardness-strain curves are fitted using the power law in Equation 1 (example shown in Figure 3b) and the prefactors ($K^*$) and exponents ($n^*$) for the power law fits are summarized in Figure 4.

5.3.1 Surface deformations (pile-up or sink-in) and underlying mechanisms

During a nanoindentation test, the material surface around the imprint can either “pile up” or “sink in”. Figure 5 shows the pile-up and sink-in effect observed in the simulations in this work. Such surface deformations are generally due to the plastic flow induced by the localized stress distribution around the indenter. For different materials or for composites with different compositions, the extent of the surface deformation (pile-up height and sink-in depth) can often be different. This difference can be attributed to the difference in the material’s composition and microstructure, which can cause the material to behave differently in terms of plastic flow and strain hardening [40]. It has been shown by data from both experiments and numerical
simulations that materials which possess higher (lower) strain hardening exponents show a lower (higher) pile-up extent (including both pile-up and sink-ins) [28].

It was found that among all the tested nanoscale metallic multilayered composites, the CuNi multilayers tend to have surface pile-ups, while CuNb multilayers tend to have surface sink-ins. However, unlike the CuNi and CuNb, the CuNiNb multilayers shows pile-up in some cases and shows sink-in other cases, the reason for this will be addressed later. See Figure 5 for examples of pile-ups and sink-ins in the multilayer systems. The pile-up heights (h>0) and sink-in depths (h<0) are measured for all test cases, they are normalized against the respective indenter radii, i.e. h/R. Recall from Figure 4(d-f), the Cu-Ni multilayers generally exhibit a lower strain hardening exponent $n$ than that of CuNb and CuNiNb, which is inverse to the relations between the multilayers for pile-up extents. Hence, to show the trend of the result better, n vs. h/R plots are used (Figure 6). In this figure, one can easily see that the observation by [28] hold for NMMs as well, i.e. the materials’ hardening exponent decrease with surface pile-up extent measured at the indentation imprint.

However, one may still wonder what caused the differences in the pile-ups extents among the different NMMs. To this end, the authors have examined the atomistic data carefully and discovered two mechanisms that are governing the surface pile-up process. (1) Surface pile-ups form as a trace of dislocations exiting the material from the surface, it is sensitive to the Burger’s vector of dislocations. (2) A portion of the surface steps formed in Cu-Ni multilayers are results of slips in \{100\} planes.

For the first mechanism, dislocations nucleate at a certain depth beneath a spherical indenter; the depth is dependent on the radius of indenter [29]. When both the leading and trailing partials
leave the top surface a full surface step forms. Given that the Burger’s vector of the dislocation is not parallel to the surface. However, this is the case only when the Burger’s vector of the full dislocation is not parallel to the interface. For instance, in all of the CuNi multilayers and some of the CuNiNb multilayers, where the full dislocations being nucleated have the Burger’s vector \( \mathbf{b} = \frac{a}{2}[011], \mathbf{b} = \frac{a}{2}[101] \) or \( \mathbf{b} = \frac{a}{2}[110], \) the pile-ups are largely due to this. Figure 7 shows this process. In Fig. 7a, the leading partial of a dislocation has a section propagated out of the top surface. This partial, followed by its trailing partial, then propagates and cross slips, leaving a full surface step behind (Fig. 7b). The later slip vector analyses [41] show that the Burger’s vector of this full dislocation is \( \mathbf{b} = \frac{a}{2}[101], \) which is non-parallel to the top surface. This dislocation propagates on the \{111\} planes. It is found that the vast majority of dislocations nucleate in CuNi are having Burger’s vectors of \( \mathbf{b} = \frac{a}{2}[101], \mathbf{b} = \frac{a}{2}[011] \) or \( \mathbf{b} = \frac{a}{2}[110], \) all of which are non-parallel to the top surface. They propagate on all \{111\} planes except for (111).

This is not the case for CuNb multilayers and other CuNiNb multilayers. Figure 8 shows the surface view of a CuNb multilayer composite during an early stage of indentation, quite a few dislocations threading within the top Cu layer are visible. Unlike CuNi, the Burger’s vector of these dislocations are \( \mathbf{b} = \frac{a}{2}[101], \mathbf{b} = \frac{a}{2}[110], \) or \( \mathbf{b} = \frac{a}{2}[011], \) which are all parallel to the top surface. The resultant surface step height is zero. Hence, no or very few surface steps are created in CuNb multilayers, the composites mainly experience sink-in.
As shown above, the nucleation and propagation of dislocations with two types of Burger’s vectors – parallel to or intersecting the top surface – dominates the plastic deformation of CuNi and CuNb multilayers (CuNiNb multilayers usually fall into one of the former two categories, as will be addressed later). For CuNi multilayers it is apparent that the Burger’s vectors of the effective full dislocations generated by the indenter are along slip directions with largest resolved shear stress (RSS) created by the indentation (the AD, BD, CD directions on the Thompson’s tetrahedron, the δD direction is the loading direction). The rest of the slip directions are perpendicular to the loading direction, thus cannot be activated. The nucleation of such dislocations is easy to comprehend.

However, for CuNb multilayers, the Burgers vectors (along AB, BC, AC directions on the Thompson’s tetrahedron) of the effective full dislocations nucleated are perpendicular to the loading direction (δD). This is counter-intuitive. Since in homogeneous media the RSS in such directions due to the indentation would be zero, there must be certain inhomogeneity responsible for nucleation of dislocations in such slip directions. According to our investigations, such inhomogeneity is the presence of the Cu-Nb (incoherent) interface. In reference to the perfect Cu and Nb crystal structures, when the KS1 Cu-Nb interface is formed, the atoms on each side of the interface rearranges, the displacement field due to such rearrangement form a periodic structure [6]. This creates a series of stress concentrations, which will be promoted upon the application of an indentation, creating a stress large enough to nucleation dislocation. In fact, for the CuNb multilayers considered in this study, dislocations always nucleate from the Cu-Nb (incoherent) interfaces (Figure 9).
The presence of the stress concentrations on the incoherent interfaces also dictates the nucleation of the effective full dislocations with Burger’s vectors being parallel to the interface/surface. Figure 10 shows the typical process of the dislocation nucleation in CuNb multilayers. The leading partial has the Burger’s vector $\mathbf{b} = \frac{a}{6} [\bar{1}21]$ (top figure), the trailing partial’s Burger’s vector is $\mathbf{b} = \frac{a}{6} [2\bar{1}1]$ (bottom figure), making the Burger’s vector of the full dislocation $\mathbf{b} = \frac{a}{2} [\bar{1}0]$, parallel to the top surface. Referring to Figure 11a, one can see that the trailing partial is determining the direction of the Burger’s vector of the effective full dislocation. If the trailing partial were to be $\mathbf{b} = \frac{a}{6} [\bar{1}12]$, then the Burger’s vector of the resulting full dislocation will intersect the top surface. Figure 11b shows the distribution of RSS on an $\{11\bar{1}\}$ plane (on which the fore-mentioned trailing partial will nucleate) along slip directions $[112]$ and $[\bar{2}1\bar{1}]$. It is clear that for the latter direction, the area of the high stress zone is considerably larger than the former one, which provide an environment more favorable for the nucleation of the partial $\mathbf{b} = \frac{a}{6} [\bar{2}\bar{1}]$.

The second mechanism is only observed in CuNi multilayers and some of the CuNiNb multilayers with larger individual layer thicknesses. This mechanism involves the reaction between two gliding dislocations (four Shockley partials) on $\{111\}$ planes, and nucleation of a new gliding dislocation on a $\{100\}$ plane as a reaction product. Figure 12 shows the typical process of this mechanism. At first a Shockley partial dislocation nucleates and propagates (Pointed by an arrow in Figure 12a). This partial has the Burger’s vector of $\frac{a}{6} [\bar{2}1\bar{1}]$ and is gliding
on the plane (\(\overline{111}\)). Then, a new Shockley partial \(\frac{a}{6}[2\overline{1}]\) nucleates on plane (111) and propagate to partial “A” (Figure 12b). A closer look can reveal that there is another partial propagating with “B” on an adjacent parallel slip plane, but this partial did not participate in the reaction being discussed here (will show later). In Figure 11c, trailing partial dislocations “C” and “D” nucleate and propagate after leadingpartials “A” and “B” respectively. Partial “C” and “D” have the Burger’s vectors \(\frac{a}{6}[\overline{1}21]\) and \(\frac{a}{6}[11\overline{2}]\) respectively. Partial dislocation “C” continue to propagate to the intersection line \(αβ\). Line \(αβ\) is the intersection line of the planes (\(\overline{111}\)) and (111), see Figure 12d. Next (see Figure 12e), partial D also propagates to line \(αβ\), and a new dislocation “E” immediately nucleates afterwards. Dislocation “E” has a Burger’s vector of \(\frac{a}{2}[0\overline{1}]\) and is gliding on plane (100). The Burger’s vector of dislocation “E” is perpendicular to line \(αβ\). In other words, this dislocation is an edge dislocation in the middle section and screw dislocations on the sides. The right portion of dislocation “E” (screw) easily cross-slipped into a (\(\overline{111}\)) plane and disassociated into two partials (red arrow in Figure 12f). The left portion of dislocation “E” (marked by green arrows in Figure 12g and Figure 12h) continued gliding for some distance and cross-slipped to another (\(\overline{111}\)) plane. This reaction can be express as following (Figure 13):

\[
\frac{a}{6}[2\overline{1}] + \frac{a}{6}[\overline{1}21] + \frac{a}{6}[2\overline{1}] + \frac{a}{6}[11\overline{2}] \rightarrow \frac{a}{2}[0\overline{1}].
\]  

(2)

This reaction involves four Shockley partial dislocations; it is interesting to compare this reaction with another dislocation reaction that involves the partial dislocations - the formation of the Lomer-Cottrell barrier. The L-C barrier is formed by the reactions of two leading partials propagating from two different \{111\} planes:
\[
\frac{a}{6}[\bar{1}2\bar{1}]+\frac{a}{6}[\bar{1}2\bar{1}] \rightarrow \frac{a}{6}[011] \quad (3)
\]

The product of this reaction is a dislocation in line [0\bar{1}1] and has a Burger’s vector of \( \frac{a}{6}[011] \).

This dislocation, also known as stair-rod dislocation, together with the two trailing partial dislocations is called Lomer-Cottrell (LC) barrier. Under extreme conditions, e.g. high compressive stress, the partial dislocation of LC lock can be pushed into the lock making the LC lock mobile again. The reaction is:

\[
\frac{a}{6}[011]+\frac{a}{6}[-211]+\frac{a}{6}[211] \rightarrow \frac{a}{2}[011], \quad (4)
\]

which is equivalent to Reaction 2.

This can be proved by artificially introducing two edge dislocations into a Cu single crystal. The dislocations are created by removing a portion of the atoms in a (011) plane (Figure 14a). Ideally, this will create a pair of full dislocations with Burger’s vectors \( \frac{a}{2}[011] \) and \( \frac{a}{2}[0\bar{1}1] \) on two (100) planes. After relaxation, however, the two full dislocations immediately dissociates into two Lomer-Cottrell barriers (Figure 14b). Then, the crystal is compressed in x direction under a constant strain rate. As the strain gradually increases, the two branches of the L-C barrier contact and full \( \frac{a}{2}[011] \) dislocations are recovered (Figure 14c). The stress level for this recovery is about 4 GPa (Figure 15a, indicated by the arrow). The structure is then sheared with gradually increased shear strain \( \tau_{xy} \). The dislocations start to move at \( \tau_{xy}=0.37 \) GPa. (See Figure 14d and Figure 15b). The plastic hardening in Figure 15b is due to the relatively high strain rate being imposed, and the dislocations are not moving fast enough to accommodate the strain. Although it
seems quite uncommon, the slip in \{100\} direction of an FCC crystal has been reported before. Tschopp et al. [42] observed a dislocation with Burger’s vector $\frac{a}{2}[011]$ gliding on a \{100\} plane which is nucleated from a $\Sigma 171$ symmetric tilt grain boundary. This nucleation was observed during a compressive loading on a Cu bicrystal, in which the loading axis was perpendicular to grain boundary. Examining the simulations mentioned above where the slip in \{100\} were observed, it can be seen that they are under quite significant compressive loads. Hence, the slip in \{100\} planes seems to be a new deformation mechanism that need to be carefully addressed in such loading conditions. In the above observations, the slip in \{100\} all seems to initiate from a specific mechanism instead of initiating from homogeneous nucleation. One can infer that the critical resolved shear stress for homogeneous nucleation of a full dislocation in \{100\} planes is very high that it seems to be impossible to observe this (homogeneous nucleation) in physically achievable loading conditions.

The surface pile-up is greatly affected by the presence of the CuNb interface. For CuNiNb multilayers, in some of the cases surface pile-up is more evident because they have relatively large individual layer thickness with combined with the fact that the Cu and Ni are on top makes the stress concentrations on the Ni-Nb interface (also incoherent, has similar stress concentrations as the Cu-Nb interface) unaffected by the indenter. Hence the material behaves more like CuNi, surface pile-up is observed. For the smaller individual layer thickness, the material behaves like Cu-Nb or Ni-Nb, surface sink-in is more evident.

5.3.2 Strain hardening and the incoherent interfaces

It is noted from Figure 4 that, the trends of variation of $K^*$ and $n^*$ of each type of multilayers (CuNi, CuNb and CuNiNb) roughly follow the same pattern with respect to the
change of individual layer thickness. For instance, when the indenter radius $R=60\AA$, as the individual layer thickness $h$ of CuNiNb drops from 50Å to 20Å, the $K^*$ of CuNiNb has a small increase at first follow by a larger increase this is very similar to the change of $n^*$ of CuNiNb. For some types of multilayers at certain $h$, $n^*$ is negative which indicate strain softening. The same observation can be made in the same type nanolayers indented by larger indenters as well as in other types multilayers. From Figure 4, it is seen that the CuNi multilayers primarily undergo strain softening, as the $n^*$ values for CuNi are negative. CuNb and CuNiNb generally have noticably higher values of $K^*$ and $n^*$, which indicates strain hardening in different degrees. Here, the multilayers that undergo strain hardening all contain Nb layers, in other words, they all contain the incoherent FCC-BCC interfaces. It suggests that the hardening effect of the incoherent FCC-BCC interfaces (Cu-Nb and Ni-Nb) in CuNb and CuNiNb nanolayers is stronger than that of coherent FCC-FCC interface (Cu-Ni) in CuNi nanolayers. This can be explained by the fact that the barrier posed by the incoherent interfaces to the gliding dislocations is stronger compared to coherent interfaces as was observed by Shao and Medyanik [15]. This can also be seen in Figres 16. The figure shows for CuNi multilayers although the partial dislocations are kinked and barricaded (indicated by black arrows) at the CuNi interfaces, they have penetrated much deeper in CuNi than they do in other multilayers (CuNiNb and CuNb) at the same indentation depth. This clearly shows that metallic interfaces and their type play a major role in hardness in the NMM composites.

One can also tell from Figure 3 that for CuNiNb and CuNb multialayers, both $K^*$ and $n^*$ decrease with the increase of the individual layer thickness $h$, while for CuNi multilayers, there are no clear trends of variation for such parameters ($K^*$ and $n^*$). This can be attributed to the density of the incoherent interfaces in the system. It has been discussed before that, the blocking
effect of Cu-Ni interface is much weaker than that of the Cu-Nb and Ni-Nb interfaces, hence, the presence of the incoherent interfaces can affect the hardening of the multilayers more significantly. For all the simulations the overall dimension of the computational cell is constant, when the individual layer thickness decreases, the number of incoherent interfaces increases, which boosted the strain hardening of the NMM composite. In addition, the decrease in individual layer thickness also result in more interfaces being affected by the high stress zone produced by the indenter, which causes the dislocations to interact with more incoherent interfaces. This is shown in Figure 16. For instance, for CuNiNb (Figures 16e-g), when $h=20\text{Å}$ the plastic zone has penetrated well through three layers, and dislocation has interacted with two incoherent interfaces - more than the case when $h=50\text{Å}$, where only two layer is involved in the plastic zone and dislocations only interact with one interface. Similar trend of variation can be observed to the CuNNb multilayers.

Form the above observations, one can conclude that amount of incoherent interface engaged in plastic deformation increases with decreasing layer thickness. Recall from Figure 4 that the parameters $K^*$ and $n^*$ also increases with decreasing layer thickness. This suggests that there must be a correlation between the parameters $K^*$ and $n^*$ and the amount of incoherent interface involved in the plastic deformation. The amount of coherent interface engaged in the plastic deformation also increases with decreasing layer thickness, however, $K^*$ and $n^*$ do not have clear tends of variation in the CuNi multilayers with respect to the varying layer thickness, which suggests that there is no relations between $K^*$ and $n^*$ and the interfacial plastic deformation. The difference between the incoherent FCC-BCC interfaces with the coherent FCC-FCC interfaces, when it comes to the plastic deformation is that, due to their low shear strength, incoherent interfaces shear to accommodate the plastic deformations, this does not
The shear deformation is carried out in the form of formation and propagation of the interfacial dislocations. It is not trivial to define dislocations in the incoherent interface since their cores spreads quite significantly, not to mention identifying them in complicated loading conditions, such as three dimensional indentation, where extensive interactions between interfacial interactions exist. However, the number of interfacial dislocation can be calculated with aid of disregistry plot developed by Hoagland et al [6]. The plot is generated by plotting the disregistry vector of each atom in the same graph. The disregistry vector is defined as: $\Delta = \mathbf{u}^+ - \mathbf{u}^-$, where $\mathbf{u}^+$ and $\mathbf{u}^-$ are displacement vectors of atoms on both sides of the interface. For a quick demonstration, the disregistry plot for a CuNi interface and a CuNb interface are shown in Figure xx and it is evident that the extent of the interfacial shear for CuNi (coherent) interface is negligible compared to that of a CuNb (incoherent) interface. It was estimated that the Burger’s vector of an interfacial dislocation in a CuNb interface is about 0.31~0.66Å [6]. Then the dislocation density contributed by a single interface $i$ ($i=1$ for the top interface, and increases as the distance between the current interface and the top surface increases) at indentation depth $d$ can be calculated as:

$$\rho_i(d) = \frac{1}{AN|\mathbf{b}|} \sum_n |\Delta_n^i|,$$

(5)

where $A$ is the vertical cross sectional area of the simulation cell, in this work $A \approx 1.6 \times 10^5 \text{Å}^2$, $N$ is the total number of atoms in the interface, $\Delta_n^i$ is the disregistry vector on $n$th atom for interface $i$, $\mathbf{b}$ is the Burger’s vector for interfacial dislocations, here $|\mathbf{b}|=0.5\text{Å}$ is used. Obviously, the greater indentation depth $d$ is, the greater interfacial shear will be. Thus $\rho_i(d)$ should also be a function of the indentation depth $d$. Hence the density of interfacial dislocations over the total volume of the simulation cell is
\[
\bar{\rho}(d) = \sum_i \rho_i(d)
\]  

(6)

The \( \rho_i(d) \) of all interfaces in each multilayer can be plotted versus their interfacial numbers \( i \). Figure 17a shows \( \rho_i \) vs. \( i \) curves for CuNb multilayers indented using indenter with radius 90Å at a indentation depth of 27Å. The dislocation density contributed by individual interfaces decreases as the position of the interface moves farther from the top surface, it decays as a power law. Similar trends are also evident for the other systems, as shown in Figure 18 shows the \( \rho_i \) vs. \( i \) curves for all the CuNb and CuNiNb multilayers. It can be noted from Figures 17 and 18, as the individual layer thickness increases, the rate of decay of \( \rho_i \) increases, which indicates that fewer interfaces are affected by the indenter. Another fact to note is that the data points are equally distributed on both sides points instead of closely grouping about the fitted curves. If they were to be connected, the result will form several zigzag lines. It was shown in [15] that the incoherent interface will shear more or less depending if it indented from the FCC or BCC side, it is believed this is the cause of the scattering of the data points observed here. The sequence of the layers of CuNb, and CuNiNb alike, is FCC-BCC-FCC-BCC… Hence, the first, third … interfaces are FCC-BCC interface, they act as if they have the indenter on the FCC side, hence shear more than the BCC-FCC interfaces who act as if the indenter is on the BCC side. The above observations can also be made for the CuNiNb multilayers.

5.4.1 A Constitutive Model for Strain Hardening in NMM from Nanoindentation Measurements

\( \bar{\rho} \), which accounts for the total interfacial shear happening within one multilayered structure, can be plotted against the individual layer thickness as shown in Figure 17b. Agreeing with the
observation made from Figure 16 before, the amount of interfacial plastic deformation (quantified using $\rho$) is decreasing with individual layer thickness $h$. This has been observed for both CuNb and CuNiNb multilayers with all thicknesses $h$ and indenter radii $R$. CuNi multilayers are excluded because they do not exhibit clear trend of variation with respect to the change of $h$, and the coherent interfaces do not experience significant plastic deformation. Recalling the reason made in the previous section: the hardening exponent $n^*$, the prefactor $K^*$ and the interfacial dislocation density all decrease with the increase of individual layer thickness $h$, it suggests that there exist certain relations between hardening parameters $n^*$, $K^*$ and total interfacial dislocation density $\rho(d)$. Such relations are shown in in Figure 19, taking $d=27\text{Å}$ as an example. The data points are fitted using power law and linear curves. It can be seen that for both CuNb and CuNiNb, $n^*$ is proportional to $\rho$, while $K^*$ is exponentially related to $\rho$ as follows.

$$n^* = n_0 \frac{\rho(d)}{\rho_0} + n,$$

$$K^* = K e^{\frac{\alpha \rho(d)}{\rho_0}}. \quad (8)$$

where $d=27\text{Å}$, $n_0$, $n$, $K$ and $\alpha$ are four fitting parameters, $\rho_0=10^{16} \text{m}^{-2}$, for CuNb and CuNiNb their values are given in Table 1. Note that there are two data points belonging to the CuNiNb data sets in each graph deviate significantly from the fitting curves in both graphs. They correspond to the parameters of CuNiNb with $h=30\text{Å}$ or $50\text{Å}$ and $R=60\text{Å}$. With such combinations of $h$ and $R$, the indenter radius is too small compared to the effective FCC layer thicknesses of $60\text{Å}$ and $100\text{Å}$ to create a high stress zone far enough to penetrate the top FCC layers to fully effect the top incoherent interfaces. Therefore, under reasonable indentation depths such as the depths in this work, these multilayers behave closer to a CuNi multilayer in the plastic regimes. In Figure 19,
we have also included the data for CuNi multilayers, which do not contain incoherent FCC-BCC interfaces and therefore no dislocations in such interfaces. Hence all data points for CuNi correspond to the interfacial shear of zero, and are located on the vertical axis. It can be seen on both graphs of Figure 19 that all the data point for CuNi fall between the y-intercepts of the fitting curves for CuNiNb and CuNb which makes sense since these points should correspond to the $K^*$ and $n^*$ values of CuNiNb and CuNb multilayers with “no interfacial shear”. It should also be noted that although the fitting parameters in Table 1 depend on the indentation depth $d$ being considered, the form of Equations 4 and 5 should be universal for all $d$ values within the plastic range considered. Then substitute Equations 4 and 5 into Equation 1 we obtain

$$\ln H^* = \ln H + \frac{\rho}{\rho_0} \ln(e^{n^* \rho_0})$$

(9)

where $H=K\varepsilon^n$, which is the conventional hardness-strain power law for nanoindentations on bulk materials. The second term on the right hand side is the correction term taking the effect of the incoherent interfaces into account.

In Figure 19, the $n^* \sim \rho$ and $K^* \sim \rho$ curves for indentations on CuNb and CuNiNb multilayers clearly deviate from each other. The CuNb multilayers demonstrate lower $n^*$ and $K^*$ at lower $\rho$ than CuNiNb, and higher values of $n^*$ and $K^*$ at higher $\rho$ than CuNiNb. Although $n^*$ and $K^*$ increase for both CuNb and CuNiNb as $\rho$ increases, they increase at different rate – the growth rate for CuNb is higher. This deviation can be attributed to the presence of both coherent and incoherent interfaces in CuNiNb multilayers, while in CuNb only incoherent interfaces are present.
For the CuNiNb multilayers, the authors have observed that the CuNi interfaces generally interact with propagating dislocations under two mechanisms. First, the partial dislocations interact with and are hindered by the CuNi interfaces similarly to what was observed in [13], as indicated by the black arrows in Figures 16h–16j. This is mainly due to the presence of opposite coherency stress in the Cu and Ni layers. Second, as a result of expansions of the stacking faults when partials propagate from Cu to Ni, a few partial dislocations can be seen having kinked (red arrows) at the CuNi interfaces. In other words, the size of the plastic zone expands from Cu to Ni. For illustration, we compare Figure 16g with Figure 16h and 16i (their effective thicknesses of the top FCC layers are very close – around 50Å). It can be seen that the width of the plastic zone (can be viewed as the distance between the bounding partial dislocations) in the Cu layer are roughly the same for the three cases, while that in the Ni layer are wider. Normally, the width of a stacking fault in Cu is usually wider than in Ni due to Cu’s lower stacking fault. Hence, the presence of the coherent CuNi interface is not the only cause of the expansion. On the other hand, the expansion happens in a setup where Ni is adjacent to the interface while Cu is on top. Thus it would make sense to consider a case where the top two FCC layers are reversed in order, i.e. NiCuNb. The result is shown in Figure 20b. Comparing to Figure 20a, it is clear that, with everything else unchanged, if the sequence of the two FCC layers is switched; the stacking faults undergo contraction instead of expansion when the partials propagate from top layer down. The difference in interfacial energies of the CuNb and NiNb interfaces is the cause for this. Thus, the interaction of the CuNi interface with dislocations in the CuNiNb multilayers is governed by the close coexistence of the coherent and incoherent interfaces.

The applied coherency stress is constant in both Cu and Ni layers, and is exerting long-range barriers to the propagation of the dislocations [5]. Hence for the first mechanism, as long as the
coherency of the interfaces is maintained, the barrier should change very little with the change of the spacing of the coherent interfaces. Also, it can be seen from Figures. 16h~16j that the expansion of the stacking faults are all evident and the extent of the expansions is not affected by the change of the individual layer thickness. Hence the barrier acting on the gliding dislocations created due to the second mechanism is not affected by the change of layer thickness, either.

On the other hand, the incoherent FCC-BCC interfaces block the propagation of dislocations under a different mechanism [6]. They pose a stress field with a shorter range. Hence, the hardening of the multilayer improves considerably with the increase of the density of incoherent interfaces. In Figure 19, the low $\bar{\rho}$ values corresponds to large spacing of incoherent interfaces (see Figure 17b). Thus in this range of $\bar{\rho}$ the contribution of the incoherent interface to the hardening of the multilayers is relatively small, and the hardening effect dominated by the CuNi interface. However, as density $\bar{\rho}$ increases, correspondingly the density of the incoherent interface in the CuNb and CuNiNb also increases, the dislocation and the hardening imposed by the incoherent interfaces becomes stronger. Also, with the change of $h$, the density of incoherent interfaces in CuNb increases approximately twice as fast as in the CuNiNb multilayers, hence $K^*$ and $n^*$ increases as fast in CuNb. As a result, the models shown in Equations (7) and (8) exhibit lower values for CuNb at low $\bar{\rho}$ and higher values of CuNiNb at high $\bar{\rho}$ as seen in Figure 19.

The contribution of the two types of the interface to the hardening of the multilayers is further analyzed in Figure 21. In the graph, Equations (7) and (8) are first plotted (solid and dashed lines in both graphs). Then, two more curves (dash dot lines) are drawn from the same intercepts the curves of CuNb, with only half of the growth rates (derivatives) of the previous curves. We assume that such curves represent the behavior of CuNiNb if “no CuNi interface were present”
(or if the adjacent Cu and Ni layers were to be replaced by single imaginary FCC layers). Then the expressions of such functions are

\[
  n^* = \frac{n_0 \overline{\rho}(d)}{2 \rho_0} + n,
\]

\[
  K^* = \frac{K}{2} (e^{\frac{\alpha \overline{\rho}(d)}{\rho_0}} + 1),
\]

where \( n_0, n, K \) and \( \alpha \) are taken from CuNb. The above argument suggests that the \( n^* - \overline{\rho}(d) \) and \( K^* - \overline{\rho}(d) \) relations of CuNiNb are the result of the superposition of the effects of coherent FCC-FCC interfaces and the incoherent FCC-BCC interfaces, and the effect of the coherent FCC-FCC interfaces can be isolated by simply subtracting contribution of the FCC-BCC interfaces from the \( n^* - \overline{\rho}(d) \) and \( K^* - \overline{\rho}(d) \) functions of CuNiNb (the dash double-dot lines in Figure 21). As can be seen, it varies very little with the change of \( \overline{\rho}(d) \).

The modified power law in Equation 9 is dependent on the indentation depth, because the measurement of \( \overline{\rho}(d) \) is greater with greater indentation depth, vise versa. If a \( \overline{\rho}(d) \) were to be measured at a different \( d \) value, all the fitting parameters \( (n_0, n, K \) and \( \alpha \) will change accordingly, although \( H \) still has the same form. Hence, it is necessary to find a parameter invariant to the loading depth \( d \) and dependent only on the geometric setup of the nanoindentation and the multilayers. We have noted: First, as mentioned previously, \( \overline{\rho}(d) \) increases with decreasing layer thickness \( h \), because more incoherent interface can engage in the plastic deformation. Moreover, the barrier acted by coherent CuNi interface to the propagating dislocations is much weaker than that created by incoherent CuNb or NiNb interfaces. Thirdly, the radius of a spherical indenter
dictates the size of high stress zone it can generate. Considering the above factors, we found that
the dislocation density in the incoherent interfaces of multilayers with individual layer thickness
at this range, i.e. 20–50 Å, is dependent on a non-dimensionalized factor $h^*/R$:

$$\bar{\rho} = f\left(\frac{h^*}{R}\right),$$  \hspace{1cm} (12)

where $h^*$ is the effective thickness of the FCC layers, e.g. if $h=20\AA$ then for CuNiNb $h^*=40\AA$,
and for CuNb $h^*=20\AA$. $R$ is the indenter radius. Figure 22 is a plot showing the $\bar{\rho}(d)$ vs. $h^*/R$
relation, using the data from all the simulations we have performed. It is found that $\bar{\rho}(d)$ and
$h^*/R$ has the following relation

$$\bar{\rho}(d) = \beta\left(\frac{R}{h^*}\right)^m.$$  \hspace{1cm} (13)

where $d=27\AA$, $m=0.7712$ and $\beta=3.512\times10^{15}(m^{-2})$, but generally $\beta$ is a function of the indendation
depth $d$. Equation (13) is then substituted into Equation (9) and yields

$$\ln H^* = \ln H + \bar{\beta}\left(\frac{R}{h^*}\right)^m \ln(e^n e^{n_0})$$  \hspace{1cm} (14)

where $\bar{\beta} = \beta / \rho_0 = 0.35$.

5.4.2 Remarks

Equation (14) suggests that the hardness of a Nb, Cu and (or) Ni based multilayers can be
predicted if the individual layer thickness and the indenter radius are given, and the range of $h$
stays within a few nano meters. The prefactor $K^*$ and the hardening exponent $n^*$ can both be
uniquely determined by giving \( h^*/R \), they both increase with increasing \( h^*/R \). Although this model only covers a very narrow range of material combinations, i.e. CuNi, CuNb and CuNiNb, we propose that the deformation mechanisms observed in this work should apply to most of the multilayers composed of FCC and BCC material with the similar stacking setup, i.e. one or more adjacent FCC layers, with one BCC layer and with KS1 FCC-BCC interfaces [9]. It is expected that the function form Equation (14) thus should also apply to such multilayers.

5.5 Summary

By performing atomistic simulations (MD and MM) of nanoindentations on nanoscale metallic multilayered composites, a series of issues of the NMM during nanoindentations have been addressed. It has been discovered that, the presence of the Cu-Nb interface plays an important role on the plastic deformation of the NMM composites – it has shown its significance in both the surface pile-up deformation and the strain hardening effect of the NMM.

In this work, the surface deformation (pile-up and sink-in) of NMM composites are closed examined. It is confirmed that for NMM, the pile-up height is inversely related to the strain hardening rate. Two surface deformation mechanisms have been discovered. The first mechanism involves the nucleation and propagation of the partial dislocations on the \{111\} planes. The second one is due to a special dislocation reaction which produces dislocations propagating on \{100\} planes. Both mechanisms are sensitive to the presence Cu-Nb interface and the distance from the interface to the top surface.

Later, the plastic deformation and strain hardening of the NMM under nanoindentations are investigated. It is found that the hardening exponent of the NMM under nanoindentation is
closely related to the shear deformation of the Cu/Ni-Nb interface. The amount of the shear deformation of such incoherent interfaces, in turn, is related to the effective thickness of the FCC layers. Hence, a constitutive model is constructed for the hardness of the NMM composites taking the indenter radii and effective FCC layer thickness as parameters.

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References:

Figure 5.1 Simulation setup of the nanoindentations in this work
Figure 5.2 Load depth curves and plastic portion of the converted hardness-strain curves of CuNi, CuNb and CuNiNb multilayers. Individual layer thickness $h=20$, 30 and 50Å, indenter radius $R=60$, 90 and 150Å.
Figure 5.3 Load depth curves and plastic portion of the converted hardness-strain curves of CuNi, CuNb and CuNiNb multilayers. Individual layer thickness $h=30\text{Å}$, indenter radius $R=90\text{Å}$
Figure 5.4 The variation of $K^*$ (a–c) and $n^*$ (d–f) with respect to individual layer thickness. The different graphs (a–c and d–f) show this variation under different indenter radii: (a & d) for $R=60\,\text{Å}$, (b & e) for $R=90\,\text{Å}$ and (c & f) for $R=150\,\text{Å}$. 
Figure 5.5 Surface pile-ups and sink-ins for CuNi, CuNb and CuNiNb multilayers during nanoindentation.
Figure 5.6 Plot of hardening exponent vs. the normalized pile-up height. $h$ is the pile-up height, $h>0$ means pile-up, $h<0$ means sink-in, $R$ is the indenter radius.
Figure 5.7. Formation of a surface step in CuNi multilayers due to the first mechanism.

Figure 5.8. Surface view of CuNb multilayer composite during an early stage of indentation. Dislocations can be seen threading with the top Cu layer.
Figure 5.9. A snapshot of the CuNb multilayers when the dislocation is nucleating from the Cu-Nb interface, top layer is Cu.

Figure 5.10. Nucleation of a trailing partial dislocation, forming an effective full dislocation with a Burgers vector \( \mathbf{b} = \frac{a}{2} \left[ \begin{array}{l} 1 \\ 1 \\ 0 \end{array} \right] \), which is parallel to the interface/surface.
Figure 5.11. Nucleation of a trailing partial dislocation. The crystallographic orientation and the resolved shear stress distribution.
Figure 5.12. Snapshots of the atomistic configuration of Cu-Ni multilayers during the formation of a surface step. Atom colored by centro-symmetric parameter. Atoms in a centro-symmetric environment are not shown.
Figure 5.13. The dislocation reaction involved in the second mechanism of the surface pile-up.

Figure 5.14. Snapshots of atomistic configuration of pure Cu during normal and shear deformation to test the mobility of $\frac{a}{2} <011>$ dislocations
Figure 5.15. Stress strain curves of the compressive loading and shear loading during the test of mobility of the dislocation gliding on a \{100\} plane.
Figure 5.16 Snapshots of atomistic configurations of CuNi (a–c), CuNb (e–g) and CuNiNb (h–j) with variable individual layers thickness (20Å, 30Å and 50Å) at indentation depth of 20Å, the indenter radius used in this figure is 90Å. Other simulations using larger indenters are not shown for brevity. In this figure, atomic defects, e.g. dislocation lines, incoherent interfaces are detected using centro-symmetry parameter (CSP) [30]. Atoms are colored as following to identify FCC interfaces: red for Cu, blue for Ni and yellow for Nb. The dislocation lines in FCC layers are all Shockley partial dislocations, the stacking faults are not shown for better visibility.
Figure 5.17 (a) plot of $\rho_i (27\text{Å})$ vs. interfacial number $i$.
(b) plot of $\bar{\rho}$ vs. individual layer thickness $h$, for $d=27\text{Å}$. 
Figure 5.18 Plots of $\rho_i(27\text{Å})$ vs. interfacial number $i$ for all CuNb and CuNiNb NMM composites.
Table 5.1 Values of fitting parameters when d=27Å

<table>
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<th>Parameters</th>
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<th>CuNiNb</th>
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<td>$n$</td>
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</tr>
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<tr>
<td>$\alpha$</td>
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<td>0.7815</td>
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</table>
Figure 5.19 Plots of exponent n* vs. total interfacial shear $\bar{\rho} (d)$ (left) and prefactor K* vs. total interfacial shear $\bar{\rho} (d)$. Where d=27Å is taken.
Figure 5.20 Snapshots of atomistic configurations of CuNiNb (a) and NiCuNb (b) indented by an indenter with radius $R=90\,\text{Å}$ at depth $d=20\,\text{Å}$. 
Figure 5.21 Demonstration of the hardening effect of CuNi, CuNb and CuNiNb interfaces with the variation of $\bar{\rho}(d)$. Here $d=27\text{Å}$ is taken as an example as before.
Figure 5.22 Plot of $\bar{\rho}$ (d) vs. $h^*/R$ when $d=27\text{Å}$. 
CHAPTER SIX: THE SPALLATION STRENGTHS OF THE CU-NI-NB- BASED
NANOSCALE METALLIC MULTILAYERS UNDER HIGH STRAIN RATE
LOADINGS
S Shao, HM Zbib, I Matorakos and DF Bahr

ABSTRACT

The Cu-Ni-Nb- based nanoscale metallic multilayers (NMM), i.e. CuNi, CuNb and CuNiNb,
under high strain rate loadings are considered in this work using molecular dynamics. The
simulations of NMMs with various individual layer thicknesses under uniaxial strains with two
different controlled strain rates are performed. The spallation mechanisms of the NMMs are
examined. The spallation strengths of the NMMs and their variations with respect to increasing
individual layer thickness are obtained and explained. The relation between the number of
available void nucleation sites and the spallation strengths are explained and verified.

6.1 Introduction

The nanoscale metallic multilayers (NMM) is a new class of composite materials which
comprise repeating metallic layers with individual layer thickness on the order of several
nanometers. This type of composites has attracted a great deal of attention in the recent years [],
the reason being they can achieve a very high strength level – on the order of the materials’
thoretical strength [1-3]. This unique feature of such materials has been generally attributed to
the interaction between single dislocations and the interfaces [4], including confined layer slip,
slip transmission, etc. This type of material has been considered in both experiments [5-6] and
numerical simulations [5-16] using different loading conditions including, uniaxial or biaxial
tension [5-9,11-12], bulge testing [5], nanoindentation [13-16], etc. The strengths [11-12], as well as the strain hardening behavior [6, 16], of the materials have been addressed. However, these investigations only focused on the low strain rate deformations, the responses of the NMM to high strain rate have seldom been considered.

In the engineering applications, the nanoscale metallic multilayers often encounter loading conditions whose strain rates fall into different ranges. Due to its dynamic and even destructive nature, materials’ response under extremely high strain rate loading conditions, i.e. shock loading, often needs to be carefully addressed. As is commonly believed, the failure of solids is usually related to the formation of voids, which then grow and coalesce with each other and form micro cracks [17]. In the context of shock loading, this process is often referred to as “spallation”. Thus, the stress level at which the spallation happens or the spall strength is a good indicator of the material strength under shock loading [18]. The spallation is determined by measuring the stress of the material the moment before spallation happens. Moreover, the spallation usually happens after excessive plasticity, e.g. propagation of dislocations, formation of stacking faults, etc.

Considerable amount of effort has been made to investigate the deformation and the damage of the materials under shock loadings [18-39]. Experimentally the shockwave is commonly generated using the Hopkinson bar [28] or the high power laser [34]. The highest strain rate that can be achieved in an experiment is about $10^7$ s$^{-1}$. However, under such a high strain rate the only information that can be extracted on the go is only the free surface velocities and displacements. The deformation and damage mechanisms of the materials, which often are in nano- or atomic scales, cannot be captured. This poses some difficulties on understanding the materials under such loading conditions. The numerical simulations, which simulate the atoms or defects
discretely, can handle such difficulties. With the capabilities of achieving a strain rate up to $10^9$-$10^{10}\text{s}^{-1}$, the simulations are reasonably close to the strain rates in the experiments. Recently, quite many numerical works studying different materials under shockwave can also be found. These materials include Cu [18-24, 26-27, 30, 33, 36], Ni [35], Al [38], Cu-Zr metallic glass [37], Pt [29], Ni-Al multilayers [39-40], diamond [31] etc. These studies address various problems from the intrinsic material response to shock, such as the shock induced plasticity [23, 26, 27, 30, 32, 33, 35, 37-38], melting [22, 29, 36, 39-40] and spallation [18-20, 34, 37], to the effect of defects on the materials’ response to shock, such as effect of vacancies or voids [19, 32, 40]. However, the material considered are mostly single crystals and even nanocrystalline materials, the nanoscale metallic multilayer is only addressed using the combination of Ni-Al [39-40]. In that work, only the melting and alloying between the Ni-Al layers are considered, the interaction between the dislocations and the interfaces are not considered. Hence, NMMs, especially the dislocation-interface interactions in NMMs and their induced spallations, are hardly considered in the context of shock loading conditions.

In this work, using molecular dynamics simulations the Cu-Ni-Nb- NMMs (including CuNi, CuNb and CuNiNb) with various individual layer thicknesses are addressed under high strain rate loadings with different strain rate. The spallation strengths of such NMMs will be obtained. The mechanisms of spallation in each type of NMMs are carefully observed and summarized. Baring such knowledge, the variations of the spallataion strengths with respect to the individual layer thickness under the different strain rates are analyzed and explained.

6.2 Simulation Details
In the fore-mentioned simulations of shock loadings, the shock deformation is often simulated using a common flyer-target setup [18-21, 39-40] (Figure 1). In this setup, a flyer and a target are modeled to impact each other at a certain relative velocity, $2u_p$, where $u_p$ is the resulting particle velocity [20]. This setup is very realistic, it simulates the actual shock loading process used in the experiment. Thus, a well defined shock front can be obtained and the magnitude and width of the shock profile can be tailored by controlling the thickness of the flyer and the relative impact velocity. However, the stress, strain-rate and temperature distribution resulting from the shock wave is highly inhomogeneous along the loading direction. Hence, this setup is suitable for extracting such material properties, as spallation strength, temperature, strain-rate, etc, for materials homogeneous along the loading direction, in which a first spallation always occurs at the highest tensile stress created by the release wave [18-21]. This topic addressed the deformation and damage of the NMMs under high strain rate deformation, which require the loading direction to be perpendicular to the metallic interfaces. A few test runs show that when NMMs are subjected to shock loading the spallations often nucleate at different spatial positions along the loading axis, see Figure 2. Due to the high inhomogeneity in the physical quantities (stress, temperature) induced by the shockwave, these positions correspond to different stress, temperature and strain rate levels, which creates difficulties in measuring such quantities of the NMMs during spallation. Hence, to better control the physical quantities in the simulation and measure the spallation strengths of the NMMs, a new setup is used in this work. Things to consider for the new setup are as follows. First, during an impact loading the spallation only happens when the local stress state is tension. Thus only tensile loading is necessary for capturing the spall damage of the NMMs [20]. Second, during an impact loading, the material does not strain in the directions perpendicular to the loading axis. Thus, uniaxial straining is the
correct boundary condition for NMMs under high strain rate [41]. Hence, in this work, the NMMs are subjected to a homogeneous strain in y direction, with controlled true strain rates, and zero strains in x and z directions, as shown in Figure 3.

The atomistic configurations include the CuNi, CuNb and CuNiNb multilayers, each of which consists about 600,000 atoms. Full periodic boundary conditions have been applied to x, y and z directions. The crystallographic orientations for the Cu, Ni and Nb layers are as follows: 

\[ x//[112]_\text{Cu}/[/\overline{1}2]_\text{Ni}, y//[111]_\text{Cu}/[/1\overline{0}]_\text{Ni}, \text{ and } z//[\overline{1}0]_\text{Cu}/[/11]_\text{Ni} \]

The interfaces formed between Cu and Ni layers are coherent interfaces, to achieve this, coherency strains have been applied to the both layers [43]. The interfaces formed between Cu and Nb, between Ni and Nb are KS1 type incoherent interface. The interatomic potentials between CuNi [43], CuNb [8] and NiNb [44] described using embedded atom method (EAM) have been used. A good amount of recent work [7, 9-10, 13-16, 45] can be found showing that such potentials have good performance when dealing with the crystallographic defects, e.g. interfaces, dislocations, vacancies, etc. The simulations are performed using an atomistic simulation package LAMMPS [46]. Prior to the loading stage, the atomistic configurations are first relaxed using molecular static and molecular dynamics simulations. The NMMs are equilibrated at temperature 10 K. Later, the uniaxial strains are applied at two different strain rates \(1 \times 10^9 /s\) and \(1 \times 10^{10} /s\) using molecular dynamics. To detect and visualize the crystallographic defects, a technique developed by Kelchner et al. called centro-symmetry parameter (CSP) is used.

### 6.3 Results and discussions

The simulations high strain rate uniaxial strain loading on CuNi, CuNb and CuNiNb multilayers with individual layer thickness of 2, 3, 5 and 7 nanometers are performed at two different strain
rates. In total, 24 simulations are performed. The obtained true stress-true strain curves are shown in Figure 4. In this figure, one can clearly see that with the lower applied strain rate, the onset of plasticity is much earlier and the maximum stress achieved is significantly reduced. Figure 4 also shows that the stress-strain curves of the NMMs under such loading conditions generally exhibit a twin peak structure, which suggests the deformation stages of NMMs. This is shown in more detail in Figures 5 and 6. When the NMMs are subjected to the high strain rate uniaxial strain loading, they NMMs usually go through three deformation stages, elastic (pre-yield), plastic (post-yield, pre-spall) and spallation (post-spall, pre-fail) (see Figure 5 using CuNiNb with individual layer thickness of 3 nm, strain rate $1 \times 10^{10}$ /s, as an example). The three deformation stages are separated by two peaks, the first peak corresponds to the onset of plasticity, the second peak corresponds to the nucleation of voids (spallation). Figure 6 shows the snapshots of CuNiNb corresponding to the three stages in Figure 5. In Stage 3, with the nucleation, growth and coalescence of the voids, the stress drops dramatically to zero. Stresses can be seen vibrating around or above zero after Stage 3, here, the materials have already failed, thus the stress-strain data can be ignored.

The yield stresses for the three types of NMMs (CuNi, CuNb, CuNiNb) generally fall into three different levels. CuNi has the highest, CuNb comes second and CuNiNb comes last. When the strain rate is changed, the yield stresses of the NMMs will be changed as a whole, the relations among them stays the same. The incoherent interface is a source of dislocations [15], thus its presence accelerates the nucleation of dislocation, hence, decreasing the yield stress. This, together with the fact that the stiffness of the high stiffness of CuNi NMM, makes the yield stresses for CuNb and CuNiNb lower than that of the CuNi. This is agreeing with the observations of the previous studies [13-16]. In CuNiNb a compressive coherency stress for Cu
and a tensile coherency stress for Ni need to be applied in the x and z directions to maintain the coherency between such layers. When uniaxial strain is applied to the NMM in y direction, the presence of the compressive coherency stress will promote the components of the deviatoric stress, thus make the yield stress of the CuNiNb lower than CuNb. It has to be noted that, the NMMs considered in this work are essentially defeat free except for the presence of the interfaces, which could result in significantly higher yield stresses compared to the real life experiments. Thus, the yield stress is not going to be considered in more detail in this work.

It can be seen that spallation happens only after severe plasticity has been developed in the materials. The spallation strengths of the NMMs under two different strain rates are summarized in Figure 7. One can easily see that the obtained spallation strengths ($\sigma_s$) of the NMM under lower strain rates are significantly lower – up to about a 2.5 GPa and about 21% difference. For some types of NMMs, e.g. CuNb, when the strain rate is changed, the trends of variation of the $\sigma_s$ stay the same. A very distinct decrease can be observed for CuNb in $\sigma_s$ as the individual layer thickness ($h$) increases for both applied strain rates. However, for the other types of NMM, the trends of variation of the $\sigma_s$ change with different strain rates. For instance, at the strain rate $1 \times 10^{10}$ /s, the $\sigma_s$ of CuNi stays about the same for different $h$ values. While at a lower strain rate, $1 \times 10^{10}$ /s, the $\sigma_s$ actually drops quite considerably with increasing $h$. Also, it was observed that among the NMMs considered in this study, spallation only happens in Cu layers, this will be shown and explained later. In the following sections, the variations of the $\sigma_s$ with respect to $h$ will be discussed for each type of NMM at two different applied strain rates.

6.3.1 The CuNb NMMs
As shown in Figure 7, the spallation strengths of the CuNb NMMs decrease as the individual layer thickness increases at both strain rates. In fact, the shape of the two curves (the two red curves in Figure 7) are almost identical, which suggests that the spallation mechanisms of the CuNi NMMs under the two strain rates are the same. The spallation mechanisms of the CuNi NMMs are further explained in Figures 8 and 9.

Figure 8 shows a typical void nucleation process using CuNb ($h = 7$ nm) under high strain rate as an example. Spallation only happens after excessive plastic deformation and the nucleation sites for voids are always the intersections of partial dislocations and the stacking faults. This is true for all NMMs considered in this study. Hence, the “ease” of the supply of the nucleation sites for void determines the spallation strengths of the NMM. The easier the NMM can supply the sites for void nucleation, the lower the spallation strength will be. Figure 9 shows the snapshots of the CuNb NMMs (with thicknesses ranging from 2 nm to 7 nm) under two strain rates. When $h = 2$ nm, the structure of the dislocation is greatly affected by the closely arranged CuNb interfaces. One can see from Figure 9 that the stacking faults have propagated through the thickness of the Cu layers and have distributed in the Cu layers very uniformly. This suggests that the partial dislocations has propagated through the Cu layers and resides within the CuNb in a parallel manner. This is due to the close coupling of the stress field [15] of the CuNb interfaces. When a partial dislocation nucleates from one CuNb interface in a Cu layer it immediately feels the stress field from the adjacent interface and is absorbed by that interface. The array of the stacking fault uniformly distributed in the Cu layer is due to the periodically distributed stress concentrations [15]. This coupling effect of the CuNb interface produced dominance in the slip planes in which the dislocations will nucleate. Thus, the nucleation of dislocations in other slip planes are suppressed which makes it difficult to form intersections between dislocations and stacking.
faults. This elevates the spallation strengths for NMMs with lower $h$. As $h$ increases, the distance between the interfaces increases, the coupling effect weakens (also visible in Figure 9). This gradually enables the nucleation of dislocations in different slip planes, which increases the amount of void nucleation site and thus reduces the spallation strengths of the CuNb NMMs with larger $h$. Also, when $h$ increases, the number of the CuNb interface decreases the dislocations tend to nucleate more frequently to accommodate for the deformation.

It is also apparent that when the strain rate is higher, the deformation of the NMM involves more dislocation nucleation. While when the strain rate is lower, the deformation involved more propagation of dislocations. The stress level for nucleating a dislocation, even with the assistance of the stress field provided by the CuNb interface, is still higher than to propagate an existing dislocation. This explains the higher $\sigma_s$ levels of the CuNb NMMs under higher strain rate. This is also true for the rest of the NMMs.

It has been reported before that under low strain rates the dislocations tend to nucleate in Cu layers from the CuNb interfaces [15]. The results in this section suggest that this hold true for NMM under high strain rates.

6.3.2 The CuNi NMMs

The $\sigma_s$ of the CuNi change differently with increasing $h$ - it stays roughly constant for low strain rate, while decreases quite noticeably for the higher strain rate. This difference can also be explained by the amount of void nucleation sites available in this type of NMM. Figure 10 shows the snapshots of CuNi in a similar manner to Figure 9. As mentioned before, due to the compressive coherency stress applied in Cu layers, the nucleation of dislocations in the CuNi NMMs only happens in Cu layers. Just like in CuNb NMMs, for the high strain rate cases, one
can see that the nucleation of dislocation is contributing to the plastic deformation. Hence, it can be observed that, in the high strain rate cases, the dislocations do not have time to propagate beyond the CuNi interface, and are all “confined” in the Cu layers. In low strain rate cases, the propagation of the dislocations is the main deformation mechanism, hence the dislocations can propagate well into the Ni layers. This is the cause of the different responses of $\sigma_s$ in CuNi NMMs with respect to $h$ under different strain rates.

At high strain rate, when $h$ is small (refer to $h=2$ and 3 for example), although the density of the dislocations is relatively high, the thickness of the Cu layer is so small that it is actually posing a geometric confinement to the width of the stacking fault (the distance partial dislocations can propagate) thus limiting the chances of the intersections between dislocation and stacking faults. Hence, the $\sigma_s$ is higher at such $h$. When $h$ increases, the limitation is gradually removed and the spallation strength drops. This is not the case for the low strain rate loading. At the low strain rate, the dislocations are propagating more freely than in high strain rates, hence does not limit the amount of sites available for void nucleation. In addition, looking at Figure 10, one can easily tell that the densities of the dislocations are roughly the same for all the $h$ in the low strain rate regime. Hence, the $\sigma_s$ levels are roughly constant in this case.

6.3.3 The CuNiNb NMMs

It is interesting to observe that the sites for nucleation of dislocations in CuNiNb NMMs are limited to CuNb interfaces. This is a fact that is expected. As explained before, the presence of the compressive coherency stress assisted the nucleation of dislocations in Cu layers especially in places close to CuNb interfaces. The presence of the tensile coherency stress in Ni gives rise to a hydrostatic tensile stress when a tensile load is applied to the NMM. This suppresses the
homogenous nucleation of dislocations inside the Ni layers, also suppresses the nucleation of dislocations in the NiNb interface.

The variation of the $\sigma_s$ in CuNiNb with respect to $h$ is different from that in CuNi and CuNb. It keeps roughly constant when loaded with higher strain rate, while decreases when loaded with low strain rate. The snapshots of the computational domain are shown in Figure 11. At the low strain rate and low $h$, the coupling effect of the incoherent interface is much weaker that of the CuNb but is still present. One factor that contributed to this is the propagation of dislocation is more tolerated in the low strain rate, hence, the dislocation nucleated from the CuNb interface still can be affected by the stress field of the NiNb interface. On the other hand, in CuNiNb multilayers, the available sites for dislocation to nucleate are almost twice as scarce as in CuNb multilayers. Hence, to accommodate the deformation under constant strain rate as the $h$ increases it is much easier to nucleate dislocations from the CuNb interface (this is especially true when the strain rate is low and homogenous nucleation of dislocation inside Cu layer is not favorable). Hence, more sites for void nucleation are created near the CuNb interface, see Figure 12. For higher strain rate, the presence of the CuNb interface assisted the propagation of the dislocations, this expands the widths of the stacking faults for low $h$ and increases the chances of intersection between stacking faults and dislocations, thus decreasing the $\sigma_s$. Also the stress field of the CuNb may also accelerate the nucleation of void at the available nucleation sites. Hence, the strength roughly unchanged. This is a contrast to CuNi at high strain rate where it decreases with increasing $h$.

6.3.4 Effect of interfacial steps in the incoherent interfaces on the spallation strengths
In the previous sections, it was observed that the voids nucleate from the intersection between a partial and a stacking fault or interaction between two partial dislocations. Under high strain rate loadings such as shock loading the material is very sensitive to the increase of the local atomic volume, because a cluster of atom with high atomic volume can serve as a nucleus of void, the growth of the void causes the spallation damage to the material. The fact that the aforementioned interactions give rise to the increase of the local atomic volume makes such locations the candidates for void nucleation. Such interactions have been illustrated in Figures 13 and 14. Figure 13 shows the two types of reactions schematically. The first type of reaction involves of two gliding partial dislocations (Figure 13a). They are all edge dislocations; their Burger’s vectors have the same magnitude $\frac{a}{6}[112]$ but opposite sense. They propagate towards each other along two adjacent (111) planes, the line vector of the partials is [110]. The two partials feel the repulsive force as move towards each other and trapped. This increases the local volume of the two dislocations cores thus provides a site for void nucleation (marked a red circle in Figure 14). Other locations for this reaction are marked by the arrows, they are at an earlier stage so the increase in the atomic volume is not yet visible. It is interesting to compare this type reaction with a similar scenario discussed by Weertman [47]. In that case, two edge dislocations moving towards each other along the same slip plane at velocities approaching sound speed pass through each other instead of annihilating. The reaction mentioned in this paper did not have pass-through is mainly due to their relatively low velocities right after the nucleation from the interface and the fact that the gliding planes are offset. The second type of reaction involves a stacking fault and a gliding partial dislocation (Figure 13b). After a partial dislocation (line vector [110]) with a Burger’s vector $\frac{a}{6}[112]$ nucleates and propagates, a stacking fault is formed.
As was mentioned in the previous sections, this type of partial dislocations is primarily nucleated from the interface. When another partial nucleates \((\frac{a}{6}[211])\) on a \((\overline{111})\) plane and intersects with the stacking fault. The local atomic volume increases at the intersection (marked by the red rectangles in Figure 14). In this work, the sites for void nucleation are generally generated by the two types of interactions explained above.

We have used the proposition that the spallation strength dictated by the number of available void nucleation sites to explain the variation of the spallation strengths of the NMMs. But it is yet to be proved until this section. Considering to fact that the voids nucleate from the interactions mentioned above, in this section we control the amount of partial dislocations to be nucleated in order to observe the effect of the number of available sites for void nucleation on the spallation strengths of the NMM. The stress concentration created by the corners of interfacial steps (or disconnections) in the incoherent interfaces are utilized as sources of dislocation nucleation [48]. Examples of the interfacial steps used in this work are shown in Figure 15, with the generation of each interfacial step two ledges are created. For both CuNb and CuNiNb multilayers, the steps are introduced into the incoherent interfaces, the number of the steps is also varied to see its effect on the spallation strength. The results are summarized in Figures 16-17. For CuNb multilayers, an individual layer thickness \(h=7\text{nm}\) is considered, different number of steps (from only 1 step over the whole volume, to 4 steps on each incoherent interface) are introduced into the NMM and compared with the case of the smooth interfaces (Figure 16). As one can see, the existence of only one or two steps in the whole NMM almost has no effect on the spallation strength (second peak) of the NMM. Because the number partial dislocations nucleated from the ledges of the step are very limited, thus does not yield a
significant increase in the number of void nucleation sites. When the number of the steps is increased to one per interface, the strength is noticeably decreased. As the number of steps is increases up to four steps per interface, the spallation strengths continued to drop. This shows that for CuNb NMM, the growth of the number of the steps increased the number of available sites for void nucleation and thus reduces the spallation strength. Things are a little more complicated for the case of CuNiNb NMM. The authors chose a CuNiNb NMM with an individual layer thickness $h=5\text{nm}$, so that the number of incoherent interfaces is the same as the CuNb NMM chosen above. As the number of steps per interfaces grows from zero to six, the spallation strength increased instead of decreasing. Interestingly, when the number continues to increase, the spallation strength starts to decrease. To explain this, one need to examine the stress fields created by the smooth and stepped incoherent interfaces in the CuNiNb NMM (Figures 18a and 18b). One can easily see that the presence of the coherency stress promotes the stress concentrations on the Cu-Nb interface and suppresses those on Ni-Nb interface (Figure 18a). What is also promoted are the stress concentrations created by the interfacial steps in Cu-Nb interfaces. Figure 18b shows the stress field of a stepped CuNiNb NMM color coded in the same range as Figure 18a. One can see that the stress field of the steps in the Cu-Nb interface is very influential and far more pronounced than the stress concentrations of a smooth Cu-Nb interface. Meanwhile, its effect is suppressed in the Ni-Nb interface due to the tensile coherency stress, down to a level comparable or weaker than a smooth Ni-Nb interface. Hence, in a stepped CuNiNb NMM, the plastic deformation is locally dominated by the ledges of the steps, which suggests that putting a few steps in the incoherent interfaces actually reduces the number of the void nucleation sites. This holds true until the number of the ledges of the steps is comparable to the number of stress concentrations in a smooth Cu-Nb interface. This is why the spallation
strength decreases for CuNiNb NMMs with more than 6 steps per interface. From 6 steps and
above, more steps actually create more void nucleation sites. Therefore the case of CuNiNb
NMM with steps also proves that the spallation strengths are closely related to the amount of
nucleation sites for voids.

6.4 Remarks

The computation cells used to model the NMMs in this work have periodic boundary conditions
applied in the loading direction. All the cells have the same dimensions. When the individual
layer thickness is varied from cell to cell, is it quite common for some cells to have one layer
(adjacent to the boundary) not having the prescribed layer thickness $h$. This is shown in Figures
19a and b. Figure 19a shows that in some cases, it is possible to have one layer with thickness
smaller than the rest of the layers. Figure 19b shows that, in some cases, when the layer with
smaller thickness is of the same atomic type as the layer on the other boundary, then due to the
periodic boundary conditions, it is possible to have a layer effectively thicker than the rest of the
layers. One may argue that such inconsistencies in the individual layer thickness may affect the
result. However, to apply the constant uniaxial strain to the cells and generate a homogeneous
strain rate field, a velocity ramp is enforced to the atoms according to their spatial position along
the loading direction. This ensures that even if early spallations happen in the layer with
abnormal thickness, the stress levels in the rest of the layers in the cell will not be altered, hence
the measurement on the spallation strengths of the NMMs will not be affected significantly. For
instance, Figure 19c shows a CuNb NMM with $h = 3$nm, the left more layer and the right most
layer are all Cu layers. Effectively this makes the combined thickness of the layer at the
boundary 6 nm. Spallation inside this layer can be observed. But the spallations in rest of the Cu
layers are very common and the spallation strength of this NMM is dominated by the spallation process occurring in such layers.

6.5 Conclusion

In this work, the Cu- Ni- Nb- based NMMs under high strain rate uniaxial loadings have been considered. The goal is to investigate the spallations damage of such NMMs happening under high strain rate shock loadings. The spallation strengths of various NMMs with various individual layers thickness under different strain rates have been measured and analyzed. The mechanisms of spallation of such NMMs have been discovered and related to the variations spallation strengths with respect to layer thickness under different strain rates. It is found that just as what has been observed before in the low strain rate testings [15], the incoherent interface is the primary source for dislocations. Without the presence of incoherent interfaces, in CuNi, the NMM primarily undergo homogeneous nucleation of dislocations in Cu layers due to the deviatoric stress generated by the coherency strain and uniaxial tensile strain. As anticipated by the dislocation nucleation theories [49], at a higher strain rate, the deformation of the NMM involves more nucleation of dislocations; at a lower strain rate, the deformation of the NMM is more likely to be accommodated by the propagation of dislocations. Due to this the barrier effect of the CuNi interfaces is stronger at higher strain rates, this can limit the width of the stacking faults thus make the nucleation of voids difficult. The close coupling of the stress field of the incoherent interfaces also can suppress the nucleation of voids. When the amount of sites for void nucleation is limited, the spallations strengths of NMMs increase. In addition, since the incoherent interfaces are the primary sources of the dislocations, when the density of the sources
decreases, the nucleation of dislocation is promoted, creating site for void nucleation, which will
decrease the spallation strength.

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Figure 6.1. A common setup for atomistic studies of shock loading

Figure 6.2. Result of a classic fly-target impact loading, taking CuNb as an example. Showing the spallation on the different spatial positions corresponding to different stress levels. Similar results can be observed for CuNi and CuNiNb as well.
Figure 6.3. The initial configuration of the NMMs.

Figure 6.4. The true stress – true strain curves of NMMs under high strain rate uniaxial strain loadings.
Figure 6.5. Defining the different deformation stages of an NMM under high strain rate loading. Using CuNiNb NMM as an example.

Figure 6.6. Illustration of the deformation stages of NMMs under high strain rate loadings, using CuNiNb NMM as an example.
Figure 6.7. The spallation strengths of the different types of NMMs with various individual layer thickness under two different strain rates.

Figure 6.8. Typical void nucleation process, using CuNb NMM as an example.
Figure 6.9. The snapshots of the CuNb NMMs right before spallation.
Figure 6.10. The snapshots of the CuNi NMMs right before spallation.

\[ \varepsilon = 1 \times 10^9 / s \]

\[ \varepsilon = 1 \times 10^{10} / s \]
Figure 6.11. The snapshots of the CuNiNb NMMs right before spallation.

Figure 6.12. Under a lower strain rate, the spallation of the CuNiNb NMMs happens near the CuNb interface in Cu layers.
Figure 6.13. The schematics for the mechanisms of the formations of the void nucleation sites. The mechanism (a) involves two partial dislocations. The mechanism (b) involves one partial dislocation and one stacking fault.

Figure 6.14. Sites for void nucleation due to the mechanisms shown in Figure 13. The circles and arrows correspond to mechanism a, the rectangles correspond to mechanism b. Color coded using centro symmetry parameter.
Figure 6.15. Example of the interfacial steps created in a CuNb multilayers (left) and a CuNiNb multilayers (right).

Figure 6.16. A comparison of stress-strain curves of the CuNb NMM with layer thickness of 7nm with different number of interfacial steps. “step0” denotes smooth interfaces, “step1” denotes one step in the whole structure, “step2” denotes two steps in the whole structure. “stepall_xn” denotes n steps per interface.
Figure 6.17. A comparison of stress-strain curves of the CuNiNb NMM with layer thickness of 5nm with different number of interfacial steps. “step0” denotes smooth interfaces, “step_xn” denotes n steps per interface.
Figure 6.18. The Von Mises stress plot of the stress field of smooth and stepped incoherent interfaces in CuNiNb multilayers. Note the stress concentrations created by the Cu-Nb interface marked using red arrows.
Figure 6.19. Due to the periodic boundary conditions and the fixed length in the initial structures of the NMMs, it is possible to have a layer with thickness smaller than the rest of the layers, see the left gray layer in (a); it is also possible to have a layer with thickness larger than the rest of the layers, see the combined white layer on the left and on the right of (b). But even with such turbulences on the boundaries, the spallation process is not affected in the majority of the NMMs, shown in (c)
CHAPTER SEVEN: SUMMARY AND FUTURE WORK
In this thesis, using the atomistic simulations, the interaction between dislocations and metallic interfaces has been visited via a material combination of Cu-Ni-Nb in two different strain rate regimes. The interfaces considered in this thesis include the coherent CuNi and incoherent CuNb and NiNb interfaces. The author hopes that materials chosen in this thesis will shed some light on the understanding of such types (coherent, incoherent) of interface in general. In the low strain rate regime, the dislocation-interface interaction is studied to investigate the strengthening effect of the interface in the plastic deformation. A 3D nanoindentation is employed as the loading technique to generate dislocations and to drive them towards the interfaces.

First, the aforementioned interaction has been treated in a rather isolated environment, where one single interface is considered each time. This allows the author to fully understand the deformation mechanisms related to an interface under the nanoindentation. The mechanisms of the plastic deformation involving the interface are observed and analyzed. The strengthening effects of the interfaces are also addressed. Then, the dislocation-interface interaction is put into a more realistic, multiple interface environment to mimic the situation that is seen in the experiments. Here, the plastic deformations of the NMMs with up to 18 interfaces under nanoindentations are analyzed. The resulting surface deformations around the indenter tip are also addressed. The mechanisms that govern the surface deformations are discovered. The interfacial dislocations residing in the incoherent interfaces are identified to be determining the strength of the NMMs. A constitutive model has been proposed based on this finding. Lastly, the dislocation-interface interaction has been considered in a high strain rate regime. The spallation strengths of the NMM has been obtained and analyzed. The effect of the interface on the spallation strengths has been investigated. The mechanisms of spallation have been observed.
The variation of the spallation strengths with respect to the individual layer thickness under two different strain rates has been explained.

The interfaces considered in this thesis include only the Cu-Ni as coherent and Cu-Nb and Ni-Nb as incoherent interfaces. As a future work, more such interfaces involving more material combinations need to be brought into consideration. Hence, a generalized understanding of the behavior of such interfaces can be formed, a generalized constitutive model for the strength of NMMs may be achieved with arbitrary material composition. As for the high strain rate regime, simulations with more strain rates need to be performed to gain a better knowledge of the NMMs under such loading conditions. Thus, the spallation strength of the NMMs can be described into a constitutive model considering the geometric factors, such as the layer thickness, and the loading factor, such as strain rate, etc.