Glide Dislocation Nucleation from Dislocation Nodes at Semi-coherent {111} Cu-Ni Interfaces

Shuai Shao^a, Jian Wang^{a,*}, Irene J. Beyerlein^b, Amit Misra^c

^aMaterials Science and Technology Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

^bTheoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

^cDepartment of Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan 48109, USA

Abstract

Using atomistic simulations and dislocation theory on a model system of semi-coherent {111} interfaces, it is shown that misfit dislocation nodes adopt multiple atomic arrangements corresponding to the creation and redistribution of excess volume at the nodes. Four distinctive node structures were identified: volume-smeared nodes with (i) spiral or (ii) straight dislocation patterns, and volume-condensed nodes with (iii) triangular or (iv) hexagonal dislocation patterns. Volume-smeared nodes contain interfacial dislocations lying in the Cu-Ni interface but volume-condensed nodes contain two sets of interfacial dislocations in the two adjacent interfaces and jogs across the atomic layer between the two adjacent interfaces. Under biaxial tension/compression applied parallel to the interface, it is shown that the nucleation of lattice dislocations is preferred at the nodes and is correlated with the reduction of excess volume at the nodes.

Keywords: atomistic simulations; dislocation; interface; nucleation.

* Corresponding author: Dr. Jian Wang, e-mail: wangj6@lanl.gov; Phone: +1 505 667 1238

1. Introduction

In metallic nanocomposites, interfaces play a dominant role in determining the deformation mechanisms that lead to ultra high strengths. Interfaces act as strong barriers for confining dislocation propagation within layers [1-7] and transmitting lattice dislocation across interfaces [8-13]. As the interface spacing decreases to a few nanometers, experimental characterization using *in situ* and *ex situ* transmission electron microscopy [14-18] indicate that lattice dislocations are likely trapped in the interfaces [4, 14]. In addition, the stress required for lattice dislocations propagation within layers significantly increases with decreasing layer thickness [19].

Much effort has been paid recently to the nucleation of lattice dislocations at interfaces and/or grain boundaries [20-28]. Dislocation nucleation from a coherent interface is difficult since it would need to overcome a high-energy barrier associated with reducing interface coherence [27, 30]. In contrast, interfacial dislocations in a semi-coherent interface, including misfit dislocations and interface disconnections, can act as sources for nucleation of lattice dislocations [25-30]. Using molecular dynamics (MD) simulations, the nucleation of lattice dislocations has been demonstrated to be related to both the characteristics of interfacial dislocations and interface properties [29, 30]. For example, a non-Schmid effect associated with dislocation nucleation was observed in Cu-Nb interfaces [28]. When multiple slip systems with the largest Schmid factors were available, only those slip systems whose slip trace was parallel to an interfacial dislocation line were activated. Salehinia *et al.* observed similar nucleation behavior in metal-ceramic Nb/NbC interfaces [31-33]. It has also been noticed that when misfit dislocation lines are not parallel to the traces of the slip planes on the interface, lattice dislocations could nucleate along dislocation junctions lying parallel to one of the slip traces and within the interface. These junctions formed via a reaction between intersecting interfacial dislocations under mechanical loading [28-30]. The interfaces in these cases were a stepped Kurdjumov-Sachs interface [30, 34, 35] or a twisted Nishiyama-Wasserman interface [36].

There are some situations in which misfit dislocation may lose the ability to nucleate lattice dislocations. For a weak-shear interface, for instance, misfit dislocations tend to have widely spread cores [8-10]. The core spreading reduces the stress or strain

concentration associated with a misfit dislocation and prevents the formation of junctions between intersecting misfit dislocations. The mechanisms of dislocation nucleation from such interfaces are not understood. The $\{111\}$ interface between two face centered cubic (fcc) crystals is an example of this kind of interface [37]. Atomistic simulations recently revealed that misfit dislocations have a wide core on the interface, particularly when the spacing between misfit dislocations approaches several times the Burgers vector and/or the coherent interface has a low shear resistance or low stacking fault energy [37, 38]. More importantly, misfit dislocation intersections (or nodes) are found to adopt multiple dislocation structures under mechanical loadings [37].

In this paper, we investigate the interfacial dislocation structures that develop under mechanical stress and dislocation nucleation from the misfit dislocation intersections (or nodes) on the Cu-Ni (111) interface with a cube-on-cube orientation relation. This work is organized as follows. In section 2, we describe the essential details of atomistic simulations and analysis methods. In section 3, we characterize the dislocation structures of a node within Cu-Ni (111) interfaces. In section 4, we examine dislocation nucleation from these nodes and discuss the corresponding nucleation mechanisms. Finally, we conclude that nodes could act as nucleation sites for lattice dislocations.

2. Methods

Molecular static/dynamics (MS/MD) simulations are carried out using the embedded atom method (EAM) interatomic potentials for Cu, Ni and their cross-pairs [39-41]. These have been shown to produce reliable results [37, 38, 42-44]. A Cu-Ni bi-crystal model containing a single Cu-Ni interface is assembled by joining two semi-infinite Cu and Ni crystals with the same crystallographic orientations and coordinates, x along $[11\bar{2}]$, y along $[111]$, and z along $[1\bar{1}0]$. The interface plane is the x - z plane. Periodic boundary conditions are applied in the x and z directions, while the semi-fixed boundary condition is applied to the y direction [10] to mimic the bulk properties of the two semi-infinite Cu and Ni crystals. To minimize the internal stresses due to the lattice mismatch, the dimensions of the simulation cell are chosen to be 16.4 nm, 10.0 nm, and 9.5 nm with respect to the x -, y -, and z -directions. The Cu-Ni bi-crystal model is first

relaxed at a temperature of 10K for 40 pico-seconds under the conditions of $\sigma_{ii}^{Cu} + \sigma_{ii}^{Ni} = 0$ ($i = x$ and z) and $\sigma_{yy}^{Cu} = \sigma_{yy}^{Ni} = 0$ and then dynamically quenched until the forces acting on each atom become less than 5 pN. Under equilibrium, the magnitude of the internal normal stresses is less than 10 MPa in the x , y and z directions. Under a finite temperature of 10K, the structures are then subjected to biaxial tension and compression parallel to the interface plane at a constant strain rate, $\dot{\epsilon} = \pm 2.5 \times 10^9/s$. During loading, a dynamics stress control is applied to ensure $\sigma_{yy}^{Cu} = \sigma_{yy}^{Ni} = 0$.

Relaxation of the interface involves two energy minimization processes [38]. First, misfit dislocation formation is associated with reducing the chemical potential of the interface via increasing interface coherence [27, 45, 46]. Second, the intersections (or nodes) between the misfit dislocations are then relaxed through local rotations and in-plane dilatation or shrinkage of the two crystals at the nodes [38]. The relaxed interface is then subject to one of two stress states, each of which can promote the nucleation of lattice dislocations from nodes into the bulk: (i) a bi-axial tensile stress and (ii) a bi-axial compressive stress, parallel to the interface plane. Such loading conditions ensure that the same Schmid factor for the equivalent slip systems on all three $\{111\}$ planes are non-parallel to the interface. Dynamic boundary conditions were adopted to achieve zero normal stress and zero shear stresses in the interface plane. We found that a node can adopt different atomic structures corresponding to mechanical perturbation, thermal fluctuation, or vacancy / interstitial absorption at a node [31-33, 37, 38, 47-49]. The details of the different node structures and dislocations nucleation are discussed in later sections.

Characterization of the dislocations both in the interface and at the nodes is accomplished via disregistry analysis [50, 51] and geometric analysis [38], although there are other methods, such as ones based on the singular values and vectors of the Nye tensor proposed by Zhang et al [52]. In the disregistry analysis, pairs of atoms that straddle the desired interface plane with the normal direction along $\vec{N}_{mnl}$ are first identified in a reference, relaxed system. The vector $\vec{r}_{ij}^r$ describes the relative position, $\vec{r}_{ij}^r = \vec{r}_i^r - \vec{r}_j^r$, between the i th atom and the j th atom that forms a pair in the reference, relaxed system where the vector $\vec{r}_i^r$ describes the position of the i th atom in the reference

system. The displacements of these atoms in the sheared system are determined with respect to the reference system. The vector $\vec{r}_{ij}^d$ describes the relative position, $\vec{r}_{ij}^d = \vec{r}_i^d - \vec{r}_j^d$, between the i th atom and the j th atom in the sheared system, where the vector $\vec{r}_i^d$ describes the position of the i th atom in the sheared system. The disregistry vector that represents slip in the interface is calculated as the projection of the difference between the two vectors on the shear plane, $\vec{d}_{ij}^a = (\vec{r}_{ij}^d - \vec{r}_{ij}^r) - (\vec{r}_{ij}^d - \vec{r}_{ij}^r) \cdot \vec{N}_{mnl}$.

In the geometry analysis (Figure 1a), due to the lattice mismatch between the Cu and Ni crystals, atoms across the interface are distinguished into three types of lattice sites: the FCC site (normal (111) stacking between the 1st Ni and 1st Cu layers, $A_{Ni}B_{Ni}C_{Cu}A_{Cu}$), an intrinsic stacking fault site (ISF, atomic stacking between the 1st Ni and 1st Cu layers, $A_{Ni}B_{Ni}A_{Cu}B_{Cu}$), and a high energy stacking fault site (HESF, atomic stacking between the 1st Ni and 1st Cu layers, $A_{Ni}B_{Ni}B_{Cu}C_{Cu}$) [38]. With this technique, a relaxed interface can be classified into four regions (Figure 1b): the FCC region, the ISF region, the misfit dislocation region separating the FCC from ISF regions, and the node region relaxed from a HESF region. Accompanying the formation of coherent interface regions (FCC and ISF), the respective crystals are subjected to uniform in-plane normal strains (i.e. ϵ_{xx} and ϵ_{zz}) in the coherent regions, tension in Ni and compression in Cu. Since the net in-plane normal strains in the two crystals are equal to zero, the misfit dislocations and the nodes will be subject to the opposite signed normal strains. With the perfect crystal as a reference, we can calculate the spatially non-uniform in-plane strains, which in turn can be characterized by the excess volume (EV).

The excess volume (EV) is calculated from a single atomic plane with one atomic-layer height of h . For a given (111) plane, a triangular mesh is constructed from atomic positions using the Delaunay triangulation algorithm (DTA) [53] (Figure 2a). The area of a triangle connecting 3 nearest neighbor atomic distances in a (111) atomic plane can be calculated as $A = A_{bulk} \cdot (1 + \epsilon_{xx}) \cdot (1 + \epsilon_{zz})$, where A_{bulk} is the area of a triangle in the (111) plane of a perfect crystal. When the bicrystal is subjected to an in-plane biaxial strain ϵ , then $A_{bulk} = \frac{\sqrt{3}}{8} a^2 (1 + \epsilon)^2$. a is the lattice constant of the FCC crystal, ϵ_{xx} and ϵ_{zz} are the normal strains in the x and z directions solely due to the presence of misfit dislocations and coherent regions. The EV is therefore represented by the volume

difference between the deformed triangle and the perfect one, referred to as ΔAh , is therefore equal to $A_{bulk}(\varepsilon_{xx} + \varepsilon_{zz} + \square\square\square\square)h$. Since the height h is unchanged, we only describe the variation of ΔA in the following sections. A positive (negative) ΔA value reflects a positive (negative) EV where the atoms are more loosely (densely) packed. The magnitude of the EV thus represents the local strain concentration. With this approach, we analyze a relaxed Cu plane and found that the integral of ΔA over the entire interface is zero, i.e. $\iint_{Interf.} \Delta A dS \equiv 0$. The normalized values of EV ($\Delta A/A_{bulk}$) corresponding to certain points of interest (such as nodes, dislocation lines, coherent areas, etc.), as well as the integration of EV for the nodes in a certain area are summarized in Table 1. The integration of EVs at a node is calculated as $\Delta A_{node} = \iint_{node} \Delta A/A_{bulk} dS$. The area represented by an atom (A_{atom}) is calculated as area of a honeycomb around an atom position (Figure 2b), and related to A_{bulk} as, i.e. $A_{atom} = 2A_{bulk}$.

3. The dislocation structures at a node

A semi-coherent (111) fcc interface contains either three sets of Shockley partial dislocations ($a/6\langle 112 \rangle$) or three sets of full dislocations ($a/2\langle 110 \rangle$), depending on the stacking fault energy [37, 38, 52, 54]. Regardless of the characters of the misfit dislocations, a node forms where misfit dislocations intersect. Under equilibrium, to maintain interface coherence when two crystals are subject to uniform normal strains, tension develops in the crystal with the smaller lattice parameter and compression in the crystal with the larger lattice parameter. Meanwhile, misfit dislocation lines or nodes form to eliminate the uniform normal strains generated in the crystals away from the interface and act as strain/stress concentrators in the interface. Using MD/MS simulation, we found that the strain concentration associated with misfit dislocation lines can be further relaxed via core spreading (although it is accompanied by a reduction in the coherent region in the interface), and the strain concentration in the node region can be further relaxed by the relative rotation and dilation/compression of the two crystals at the node. The dilation/compression is responsible for the creation of the EV at a node, in which a positive EV in the crystal with the larger lattice parameter and a negative EV in the crystal with the smaller lattice parameter. From the viewpoint of dislocation theory,

such EV could be associated with the formation and climb of dislocation jogs [37, 49, 50].

Under bi-axial straining, we observed four distinctive node structures. According to the distribution of the excess volume and the nodal dislocation structure, we define them as: volume-smeared nodes with (I) spiral or (II) straight dislocation patterns and volume-condensed nodes with (III) triangular and (IV) hexagonal dislocation patterns. In what follows, we describe the dislocation structures of these nodes and the corresponding formation mechanisms.

(I) Structure I: volume-smeared node with spiral dislocation pattern.

A volume-smeared node with spiral dislocation pattern (Figure 3a) forms when the bi-crystal is relaxed at low temperature and zero applied stresses. Driven by the reduction of the node energy and dislocation's self-energy, the dislocation lines are not parallel to the traces of the (111) slip planes [37, 38]. Corresponding to a relaxed semi-infinite bi-crystal, a unit cell of the interface is comprised of different numbers of atoms from both crystals. The crystal with a small lattice contains more atoms than the crystal with a large lattice. During relaxation, coherent interface regions form (marked by blue regions in Figure 3b). Atoms not present in the coherent region are located at misfit dislocation lines and nodes (red regions in Figure 3b) and act as strain contractors within the interface and generate strain fields in both crystals away from the interface to eliminate uniform normal strains associated with interface coherence. Figures 3c and 3d show the plot of excess volume in the nodal area on both Cu and Ni sides of the interface. For the Cu crystal, the positive EVs are present at the nodes (white, $\Delta A/A_{\text{bulk}}=0.158$) and along the misfit dislocation lines (light blue, $\Delta A/A_{\text{bulk}}=0.025$), while the negative EVs are present in the coherent interface regions (dark blue, $\Delta A/A_{\text{bulk}}=-0.028$). For the Ni, the negative EVs are present at a node (dark blue, $\Delta A/A_{\text{bulk}}=-0.069$) and along the misfit dislocation lines (light blue, $\Delta A/A_{\text{bulk}}=-0.019$), while the positive EVs are found in the coherent interface regions (white, $\Delta A/A_{\text{bulk}}=0.022$). Via integration of EVs within a 3 nm radius of the node, we find that $\Delta A_{\text{node}}/A_{\text{bulk}}$ is 17.851 and corresponds to the area of 9 atoms in the atomic plane (111) of Cu. Note that the magnitude of EVs on the Ni side is significantly smaller than on the Cu side of the node due to its higher elastic constants.

We use solid black lines to separate the regions with positive EV from those with negative EV.

(II) Structure II: volume-smeared node with straight dislocation pattern.

When the relaxed Structure I is subject to a biaxial in-plane compression, its spiral pattern disappears and the misfit dislocation lines become aligned with the traces of the (111) slip planes (Figure 4a). This is observed when the in-plane biaxial strain reaches -0.058. More importantly, the dimensions of the dislocation cores and the nodes are significantly greater than those of Structure I. Consequently, the strain energy at the node decreases but the chemical potential at the node increases due to the loss of some area of interfacial coherence. Because of the wider core the strain concentration at the node and along the misfit dislocations decreases. This reduction is also reflected by the reduction in the EV at the nodes and along the dislocations. Figures 4c and 4d are the contour plots of the EV in the vicinity of the node on both the Cu and Ni sides of the interface. As summarized in Table 1, the EV at the node and along the dislocations on the Cu side are $\Delta A/A_{\text{bulk}}=0.142$ and $\Delta A/A_{\text{bulk}}=0.025$, respectively. The integration of EVs within a 3 nm radius of the node is $\Delta A_{\text{node}}/A_{\text{bulk}}=15.503$ and corresponds to the area of 8 atoms in atomic plane (111) in Cu. All these are considerably smaller in magnitude than those in Structure I (the volume-smeared node with spiral dislocation pattern). While on Ni side, the EV along the dislocation lines is reduced in magnitude by a factor of 2 with respect to Structure I associated with the core spreading of misfit dislocations, indicating a decrease in strain concentration along the misfit dislocation and loss of interface coherence.

(III) Structure III: volume-condensed node with triangular dislocation pattern.

When the bi-crystal with Structure I is subjected to biaxial in-plane stretching, the core of the misfit dislocations and the node regions condense into a narrow region. This is ascribed to the increase of interface coherence due to the increased amplitude of the generalized interface stacking fault profile [38]. This structure is observed when the in-plane biaxial strain reaches 0.041 and is designated as Structure III(a) (Figure 5). As shown in Table 1, the magnitudes of EV along the misfit dislocations are 0.036 on the Cu side and 0.029 on the Ni side, being significantly higher than those of Structures I and II (0.025 and 0.0009 on Cu, -0.019 and -0.009 on Ni). Very noticeably, the maximum EV at the node on the Cu side is 0.68, more than four times higher than that in Structures I

(0.158) and II (0.142). These trends suggest a high strain concentrator can be associated with the nodes and misfit dislocations in Structure III(a).

The high strain concentration or the condensed EV at the node on the Cu side can be further relaxed via the climb of three jogs along the $\langle 110 \rangle$ directions (Figure 6). The three jogs connect two sets of interfacial dislocations in the two adjacent planes Ni1-Cu1 (between the Cu and the Ni crystals) and Cu1-Cu2 (between the first and second atomic planes in the Cu crystal). Because the two sets of interface dislocation structures are only one atomic plane apart, the EV induced by the jogs is confined in the Cu1 atomic plane. Therefore, the EV calculation on Cu side of these structures is performed on the Cu1 atomic plane only. Figure 6c shows the dislocation structure. Each of the two planes contains three full dislocations with opposite Burgers vectors. Such dislocation structures at the node can also happen due to the absorption of interstitials (Figure 6) at a node or a mechanical perturbation (Figure 7) [37]. As observed in MD simulations, the node with the separated jogs is referred to as the triangular dislocation pattern. Thus Structure III(a) can be regarded as the close clustering of the three jogs seen in the projected view in Figure 5c, as each of the jogs contains certain amounts of EV. The extended structures are thus designated as Structure III(b) as shown in Figure 6, which is induced by a point defect and as Structure III(c) in Figure 7, which is induced by mechanical perturbation. Once Structures III(b) and III(c) form, we examined the stability of these structures by applying inverse loading back to a zero stress state [35]. Table 1 shows that the separation of the three jogs has indeed relieved the stress concentration caused by the EV at the center of the node, i.e. the maximum EV at the node on Cu side is 0.299 and 0.336 for Structures III(b) and III(c), respectively, as opposed to 0.680 for Structure III(a).

(IV) Structure IV: volume-condensed node with a hexagonal dislocation pattern.

Triangular nodes (Structure III) can transform into an expanded hexagonal structure (Figure 8a-b) when it is relaxed at a finite temperature of above 10 K. Interestingly, similar extended hexagonal node structures had been observed in experiments [47, 55]. Figure 8c illustrates how the structure is transformed from Structure III via the following dislocation operation. On the Ni1-Cu1 plane, the partial edge dislocations (blue and purple) react and form the full dislocations segments marked in red. The segmental partial/full dislocations on the Ni1-Cu1 plane align with the

segmented partial dislocations on the Cu1-Cu2 plane to form low-energy configurations. As a result, six superior dislocations are created and enclose the central extrinsic stacking fault region. The superior dislocation here means that two dislocations on the adjacent glide planes form a double-core dislocation [56]. Three of these combine perfect-partial dislocations (e.g., CB-C δ , AC-A δ , BA-B δ) and three others combine partial-partial dislocations (e.g., A δ -C δ , B δ -A δ , C δ -B δ). It is apparent that the dislocation segments with the full-partial combination correspond to the regions with a high EV of 0.658 in Figure 8a, while the dislocation segments with the partial-partial combination have a small EV of 0.041. The node structure presented in Figure 8 has transformed from the Structure III(b), which formed via the absorption of one interstitial. Therefore, the integration of EVs at the node in Structure IV is 17.676, which is consistent with the node Structure III(b) (17.084), and noticeably smaller than those of Structures III(a) and (c) (18.080 and 18.928, respectively). The differences are respectively, 0.996 and 1.844, which correspond to roughly the area occupied by one interstitial in the $\{111\}$ plane.

4. Dislocation Nucleation at nodes

4.1 Nucleation mechanisms

Under in-plane tension, the volume-smeared nodes with a spiral dislocation pattern (Structure I) will transform into volume-condensed nodes with either triangular (Structure III) or hexagonal (Structure IV) dislocation patterns. While under in-plane compression, they will transform into the volume-smeared node with a straight dislocation pattern (Structure II). Therefore, the nucleation of lattice dislocations at the (111) cube-on-cube interface can be categorized into three groups, i.e. (1) nucleation at the volume-condensed nodes with a triangular dislocation pattern, (2) nucleation at the volume-condensed nodes with a hexagonal dislocation pattern, and (3) nucleation at the volume-smeared nodes with straight dislocation pattern. In what follows, we discuss nucleation mechanisms of lattice dislocations from these nodes with respect to their structure.

(1) Nucleation at the volume-condensed nodes with triangular dislocation pattern

Under biaxial tension, we observed the nucleation of three Shockley partial half-loops simultaneously into three $\{111\}$ planes of Cu layer ((α) , (β) , and (γ) planes in

Figure 9a. Using disregistry analysis, we characterized these dislocations and the change in dislocation structure in the vicinity of the node. Figure 9b illustrates the node structure after dislocation nucleation. The Burgers vectors of the partial loops (marked in red) are determined to be αB along CB on the plane (α), βC along AC on the plane (β), and γA along BA on the plane (γ). They are indeed equivalent with the same Schmid factor of 0.157 (Table 2). After the emission of the partial dislocations, three stair-rods ($\delta\alpha$, $\delta\beta$ and $\delta\gamma$) form. The stair-rods, the emitted partial dislocations, together with the interfacial dislocations $A\delta$, $B\delta$, and $C\delta$, form three Lomer-Cottrell junctions, i.e. $\alpha B-\delta\alpha-A\delta$, $\beta C-\delta\beta-B\delta$, and $\gamma A-\delta\gamma-C\delta$.

A detailed look at the inception of nucleation reveals the exact nucleation sites. Figure 9c-d shows the atomic monolayer on Ni side of the interface at the node right before and during the nucleation. Since the interface stacking fault energy increases when the bi-crystal is subject to biaxial tension, the ISF regions decrease, as shown in Figure 9c. Under the influence of thermo fluctuation and tensile stress, the dislocation arms $C\delta$ and δA can temporarily recombine into a short segment of a full mixed dislocation CA (bright red in Figure 9d) near the node. This newly formed dislocation segment CA is along BA and parallel to the trace of the (γ) plane. Due to the three fold symmetry of the node structure, two more segments of the same kind form. The nucleation then happens along these segments. After the nucleation, the residual interfacial dislocation re-dissociates into a partial ($C\delta$) and a stair rod dislocation ($\delta\gamma$). The nucleation process greatly reduces the excess volume at the node, i.e., reducing the strain concentration at the node. Figures 9e-f show the comparison of excess volume at the node before and after the dislocation nucleation. It is evident that the magnitude of the excess volume associated with the jogs (0.628 in Figure 9e) is significantly reduced (peak value of only 0.336 in Figure 9f). The integration of EVs within a 3 nm radius of the node on structure III(b) right before and right after the nucleation also experiences a significant reduction, from 17.129 to 9.372, which suggests the redistribution of EV from the node to the freshly nucleated lattice dislocations and the reduction of the strain concentration at the node.

On each of the three $\{111\}$ slip planes that are non-parallel to the interface (planes (α), (β) and (γ)), there are three leading Shockley partial dislocations. Under

biaxial tension, two of them have the same, positive Schmid factor of 0.157 and the third one has the negative Schmid factor of -0.314 (Table 2). As a result, the two slip systems with the positive Schmid factor could be activated. However, MD simulations only reveal the nucleation on one of them. We thus further examine whether part of the Burgers vector of the interfacial dislocation can be released associated with the nucleation of lattice dislocation. According to our previous study [29], if $b_{ID} \cdot b_{LD} > 0$, the nucleation will release part of the Burgers vector of the interface dislocation, where b_{ID} is the Burgers vector of interfacial dislocation and b_{LD} is the Burgers vector of the nucleated lattice dislocation. Table 2 lists the value of $b_{ID} \cdot b_{LD}$ for all possible slip systems. It is clearly shown that only one of the two slip directions with positive Schmid factor on each slip plane has $b_{ID} \cdot b_{LD} > 0$. Thus, the preferred nucleation is associated with the partial αB on the plane (α) along CB, the partial βC on the plane (β) along AC, and the partial γA on the plane (γ) along BA. This agrees with MD results.

(2) Nucleation at the volume-condensed nodes with hexagonal dislocation pattern

Under biaxial tension, dislocation nucleation was observed from the extended hexagonal node structures. Before nucleation of lattice dislocations, interfacial dislocation segments near the node temporarily recombine and form perfect dislocation segments (red shaded regions in Figure 10a). The recombined dislocation segments align with the traces of the $\{111\}$ planes (along AB/BA, BC/CB and CA/AC) and act as nucleation sites. Among the slip systems with positive Schmid factors, we further compare the dot product of the lattice dislocation and the interfacial dislocation. With the results of $b_{ID} \cdot b_{LD} > 0$, the following dislocations can be nucleated: the partial dislocation $C\alpha$ on the plane (α) along BC, the partial dislocation $A\beta$ on the plane (β) along CA and the partial dislocation $B\gamma$ on the plane (γ) along AB. Disregistry analysis of the atomic structure shown in Figure 10b reveals the Burgers vectors of the three Shockley partial dislocations (Figure 10c), that are consistent with the theoretical analysis. The nucleation relieved the strain concentration (or excess volume) at the node. Figure 10d-e shows the contour plots of EV at node before and after the nucleation event. It is noted that the regions with high EV are scattered and have smaller area compared to that before nucleation. As a result, the integration of EVs within a 3 nm radius of the

node experiences a significant reduction from 18.141 to 10.826 after the nucleation of lattice dislocations.

(3) Nucleation at the volume-smeared nodes with straight dislocation pattern

Under biaxial compression, the disappearance of the spiral pattern realigns the dislocations lines with the traces of the $\{111\}$ slip planes (AB/BA, BC/CB and CA/AC directions, Figure 11a). The dislocation lines are expected to be the primary sources of dislocation nucleation. Due to the relatively high stress concentration at the nodes [38], lattice dislocations may nucleate from the straight misfit dislocation lines near the node. As expected, our MD simulations reveal the simultaneous nucleation of six Shockley partials from all of six misfit dislocation segments near the node (Figure 11b). Different from that under biaxial tension, only one of the three partial slip directions on each $\{111\}$ slip plane under the biaxial compression has a positive Schmid factor (Table 3). They are αD on (α) , βD on (β) and γD on (γ) , and they have a Schmid factor of 0.314. Moreover, their dot product with the interfacial dislocations satisfies $b_{ID} \cdot b_{LD} > 0$.

Disregistry analysis confirms the above prediction. The characterized dislocation structure is shown in Figure 11c. The freshly nucleated dislocations are marked in Red, which are the partial $D\alpha$ along the CB direction and the partial αD along the BC direction on the plane (α) , the partial $D\beta$ along the AC direction and the partial βD along the CA direction on the plane (β) , the partial $D\gamma$ along BA direction and partial γD along AB direction on the plane (γ) . After the partial dislocation loops nucleate, they propagate, react with neighboring loops and form three stair-rod dislocations (in Figure 11d, marked in dark red). Note that this perfectly symmetric dislocation structure may not always be the case as under thermal fluctuations the partials may propagate under different rates. This nucleation mechanism also decreases the EV at the smeared node (Figure 11e). The maximum value of EV is reduced to 0.125 from 0.142 of Structure II. The integration of EVs at the node within a 3 nm radius of the node after dislocation nucleation is significantly reduced from 15.503 to 7.075. The excess volume plot is generated from the positions of the Cu interface atoms projected onto the interface. Therefore, the atoms in the interface steps are projected onto the interface plane and cause the “strips” of negative excess volume (dark blue) in the plot. This explains why the integration of EVs at the node is noticeably smaller than that for Structures III (9.372) and IV (10.826).

5. Summary

In this work, using the Cu-Ni cube-on-cube {111} interface as an example, we have demonstrated the transformation of dislocation structures at a node under thermal fluctuations and applied stress, and the mechanism of glide dislocation nucleation from nodes.

We have discovered that the nodes transform into different structures under thermal, mechanical and atomic perturbations. Under equilibrium conditions, a node has smeared excess volume and the dislocation lines spiral around the node. Under biaxial compression parallel to the interface, the dislocation lines coming out of the node straighten, while maintaining the smeared excess volume. Under biaxial tension, however, the excess volume at a node concentrates, represented by three closely clustered jogs. The jogs connect two sets of interfacial dislocations on the two adjacent planes, and the node assumes a triangular dislocation structure. With the aid of thermal fluctuations and/or mechanical perturbation, the jogs can climb along the $\langle 110 \rangle$ directions. The triangular node with separated jogs can also be obtained by the addition of interstitials. Under biaxial tension, a triangular node can also jump into a hexagonal dislocation structure. All six segments of the hexagon have superior dislocation structure: three segments are partial-partial type and others are perfect-partial type. The excess volume concentrates at the perfect-partial dislocations segments. As such, the fundamental description of the transformation of the dislocation structures at a node is merely associated with the creation and redistribution of excess volume. The generalized interfacial stacking fault energy profile affects the transformation of the nodal structures. As was discussed in Ref. [38], the minimization of the interface chemical energy expands the coherent regions therefore constricting the core size of the interface dislocations and nodes. As a result, the excess volume is more condensed and pronounced in the core regions when the amplitude of the generalized stacking fault energy profile increases. Therefore, the spiral pattern of the Structure I is more pronounced. Also the nodes with Structure I is more easily transformed into the triangular (Structure III) and hexagonal (Structure IV) structures. Under compression, the increased generalized stacking fault energy profile means the transformation from Structure I to Structure II is difficult. On the other hand, if the generalized stacking fault energy profile [38] is reduced, the inverse

is true. The bulk stacking fault energy also affects the transformation of the nodal structures. The Structures III and IV involve dislocations in Cu and an extrinsic stacking fault is formed in the center in such structures. Naturally, higher stacking fault energy in Cu does not favor the transformation from Structure I to Structures III and IV.

Dislocation nucleation is a thermally activated process. Correspondingly a high strain/stress concentrator will be a preferred nucleation site/source under mechanical loading. At a semi-coherent interface, the nodes and misfit dislocations often act as strain/stress concentrators and the corresponding nucleation mechanisms are correlated with their atomic structures. The nucleation mechanisms and processes explored from atomistic simulations are able to provide insight into the characteristics of interface dislocations and their nodes, as well as correlate dislocation nucleation with interfacial dislocation structures [30, 57].

In this work, we explored the significant impact of the various node structures on lattice dislocation nucleation. For the triangular and the hexagonal node structures with concentrated excess volume, the interfacial dislocations with Burgers vector $1/6\langle 112 \rangle$ near the nodes can temporarily recombine and form full dislocations segments with Burgers vector $1/2\langle 110 \rangle$. Such segments align with the traces of the slip plane and serve as nucleation sources for lattice dislocations. For volume-smeared nodes with a straight dislocation pattern, the interfacial dislocation segments are parallel to the traces of the slip systems. The interface dislocation segments near the node serve as nucleation sources. Despite the various nucleation mechanisms of the lattice dislocations, two fundamental conditions must be satisfied if a nucleation event was to happen: (1) the interfacial dislocation that serves as nucleation sources/sites must align with the slip trace, and (2) the dot product of both Burgers vectors of the nucleated lattice dislocation and the interfacial dislocation must be greater than zero, thereby relieving the associated strain/stress concentration after the nucleation. In addition, all the nucleation events are accompanied by reduction of excess volume at the node, this suggests that the nucleation of the lattice dislocation relieves the strain concentration at the nodes and/or redistributes the EV to the freshly nucleated dislocations. In future, the dislocation reaction rules inferred from atomistic models can be incorporated into meso-scale dislocation dynamics

models to explore the evolution of interfacial dislocation network and the activity of interface dislocations during mechanical deformation at large scale [58-60].

Acknowledgement: SS, JW, and AM acknowledge the support provided by the US Department of Energy, Office of Science, Office of Basic Energy Sciences. SS and IJB also thank the support provided by the Center for Materials at Irradiation and Mechanical Extremes, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Grant No. 2008LANL1026. JW also acknowledges support provided by the Los Alamos National Laboratory Directed Research and Development (LDRD-ER20140450). The valuable discussion with Prof. J.P. Hirth, Richard G. Hoagland, and Robert Pond is appreciated.

References

- [1]. A. Misra, J.P. Hirth, H. Kung, Single-dislocation-based strengthening mechanisms in nanoscale metallic multilayers, *Phil. Mag. A* 82 (2002) 2935-2951.
- [2]. J. Wang, A. Misra, Strain hardening in nanolayered thin films, *Curr. Opin. Solid State Mater. Sci.* 18 (2014) 19-28.
- [3]. A. Misra, J.P. Hirth, R.G. Hoagland, Length-scale-dependent deformation mechanisms in incoherent metallic multilayered composites, *Acta Mater.* 53 (2005) 4817-4824.
- [4]. N. Li, J. Wang, A. Misra, J.Y. Huang, Direct observations of confined layer slip in Cu/Nb multilayers, *Microsc. Microanal.* 18 (2012) 1155-1162.
- [5]. P.M. Anderson, T. Foecke, P.M. Hazzledine, Dislocation-based deformation mechanisms in metallic nanolaminates, *MRS Bull.* 24 (02) (1999) 27-33.
- [6]. Q. Li, P.M. Anderson, Dislocation-based modeling of the mechanical behavior of epitaxial metallic multilayer thin films, *Acta Mater.* 53 (2005) 1121-1134.
- [7]. J.S. Carpenter, A. Misra, P.M. Anderson, Achieving maximum hardness in semi-coherent multilayer thin films with unequal layer thickness, *Acta Mater.* 60 (2012) 2625-2336.
- [8]. J. Wang, R.G. Hoagland, X.Y. Liu, A. Misra, The influence of interface shear strength on the glide dislocation–interface interactions, *Acta Mater.* 59 (2011) 3164-3173.
- [9]. J. Wang, R.G. Hoagland, J.P. Hirth, A. Misra, Atomistic simulations of the shear strength and sliding mechanisms of copper–niobium interfaces, *Acta Mater.* 56 (2008) 3109-3119.
- [10]. J. Wang, R.G. Hoagland, J.P. Hirth, A. Misra, Atomistic modeling of the interaction of glide dislocations with “weak” interfaces, *Acta Mater.* 56 (2008) 5685-5693.
- [11]. A. Misra, M.J. Demkowicz, J. Wang, R.G. Hoagland, The multiscale modeling of plastic deformation in metallic nanolayered composites, *JOM* 60 (4) (2008) 39-42.

- [12]. P.M. Anderson, Z. Li, A Peierls analysis of the critical stress for transmission of a screw dislocation across a coherent, sliding interface, *Mater. Sci. Eng. A* 319-321 (2001) 182-187.
- [13]. Y. Shen, P.M. Anderson, Transmission of a screw dislocation across a coherent, non-slipping interface, *J. Mech. Phys. Solids* 55 (2007) 956-979.
- [14]. N. Li, J. Wang, J.Y. Huang, A. Misra, X. Zhang, In situ TEM observations of room temperature dislocation climb at interfaces in nanolayered Al/Nb composites, *Scripta Mater.* 63 (2010) 363-366.
- [15]. N. Li, J. Wang, A. Misra, X. Zhang, J.Y. Huang, J.P. Hirth, Twinning dislocation multiplication at a coherent twin boundary, *Acta Mater.* 59 (2011) 5989-5996.
- [16]. J. Wang, N. Li, O. Anderoglu, X. Zhang, A. Misra, J.Y. Huang, J.P. Hirth, Detwinning mechanisms for growth twins in face-centered cubic metals, *Acta Mater.* 58 (2010) 2262-2270.
- [17]. N. Li, J. Wang, J.Y. Huang, A. Misra, X. Zhang, Influence of slip transmission on the migration of incoherent twin boundaries in epitaxial nanotwinned Cu, *Scripta Mater.* 64 (2011) 149-152.
- [18]. N. Li, J. Wang, X. Zhang, A. Misra, In-situ TEM study of dislocation-twin boundaries interaction in nanotwinned Cu films, *JOM* 63 (9) (2011) 62-66.
- [19]. J. Wang, A. Misra, An overview of interface-dominated deformation mechanisms in metallic multilayers, *Curr. Opin. Solid State Mater. Sci.* 15 (2011) 20-28.
- [20]. R.G. Hoagland, S.M. Valone, Emission of dislocations from grain boundaries by grain boundary dissociation, *Phil. Mag.* 95 (2015) 112-131.
- [21]. D.E. Spearot, M.A. Tschopp, K.I. Jacob, D.L. McDowell, Tensile strength of $\langle 100 \rangle$ and $\langle 110 \rangle$ tilt bicrystal copper interfaces, *Acta Mater.* 55 (2007) 705-714.
- [22]. M.A. Tschopp, D.E. Spearot, D.L. McDowell, in: J.P. Hirth (Ed.), *Dislocations in Solids Vol. 14*, Elsevier B.V., Amsterdam, 2008, pp. 43-139.
- [23]. M.A. Tschopp, G.J. Tucker, D.L. McDowell, Atomistic simulations of tension-compression asymmetry in dislocation nucleation for copper grain boundaries, *Comp. Mater. Sci.* 44 (2008) 351-362.
- [24]. M.A. Tschopp, D.L. McDowell, Grain boundary dislocation sources in nanocrystalline copper, *Scripta Mater.* 58 (2008) 299-302.
- [25]. J. Wang, R.F. Zhang, C.Z. Zhou, I.J. Beyerlein, A. Misra, Interface dislocation patterns and dislocation nucleation in face-centered-cubic and body-centered-cubic bicrystal interfaces, *Int. J. Plast.* 53 (2014) 40-55.
- [26]. R.F. Zhang, J. Wang, I.J. Beyerlein, T.C. Germann, Dislocation nucleation mechanisms from fcc/bcc incoherent interfaces, *Scripta Mater.* 65 (2011) 1022-1025.
- [27]. R.F. Zhang, J. Wang, I.J. Beyerlein, A. Misra, T.C. Germann, Atomic-scale study of nucleation of dislocations from fcc-bcc interfaces, *Acta Mater.* 60 (2012) 2855-2865.
- [28]. I.J. Beyerlein, J. Wang, R.F. Zhang, Interface-dependent nucleation in nanostructured layered composites, *APL Mater.* 1 (2013) 032112.

- [29]. I.J. Beyerlein, J. Wang, R.F. Zhang, Mapping dislocation nucleation behavior from bimetal interfaces, *Acta Mater.* 61 (2013) 7488-7499.
- [30]. J. Wang, C.Z. Zhou, I.J. Beyerlein, S. Shao, Modeling interface-dominated mechanical behavior of nanolayered crystalline composites, *JOM* 66 (1) (2014) 102-113.
- [31]. I. Salehinia, S. Shao, J. Wang, H.M. Zbib, Interface structure and the inception of plasticity in Nb/NbC nanolayered composites, *Acta Mater.* 86 (2015) 331-340.
- [32]. I. Salehinia, S. Shao, J. Wang, H.M. Zbib, Plastic Deformation of Metal/Ceramic Nanolayered Composites, *JOM* 66 (10) (2014) 2078-2085.
- [33]. I. Salehinia, J. Wang, D.F. Bahr, H.M. Zbib, Molecular Dynamics Simulations of Plastic Deformation in Nb/NbC Multilayers, *Int. J. Plast.* 59 (2014) 119-132.
- [34]. S.B. Lee, J.E. LeDonne, S.C.V. Lim, I.J. Beyerlein, A.D. Rollett, The five-parameter Heterophase Interface Character Distribution (HICD) of physical vapor-deposited and accumulative roll-bonded Cu-Nb multilayer composites, *Acta Mater.* 60 (2012) 1747-1761.
- [35]. J.S. Carpenter, X. Liu, A. Darbal, N.T. Nuhfer, R.J. McCabe, S.C. Vogel, J.E. LeDonne, A.D. Rollett, K. Barmak, I.J. Beyerlein, N.A. Mara, A comparison of texture results obtained using precession electron diffraction and neutron diffraction methods at diminishing length scales in ordered bimetallic nanolamellar composites, *Scripta Mater.* 67 (2012) 336-339.
- [36]. J. Wang, R.F. Zhang, C.Z. Zhou, I.J. Beyerlein, A. Misra, Characterizing interface dislocations by atomically informed Frank-Bilby theory, *J. Mater. Res.* 28 (2013) 1646-1657.
- [37]. S. Shao, J. Wang, A. Misra, R.G. Hoagland, Spiral Patterns of Dislocations at Nodes in (111) Semi-coherent FCC Interfaces, *Sci. Rep.* 3 (2013) 2448.
- [38]. S. Shao, J. Wang, A. Misra, Energy minimization mechanisms of semi-coherent interfaces, *J. App. Phys.* 116 (2014) 023508.
- [39]. Y. Mishin, M.J. Mehl, D.A. Papaconstantopoulos, A.F. Voter, J.D. Kress, Structural stability and lattice defects in copper: *Ab initio*, tight-binding, and embedded-atom calculations, *Phys. Rev. B* 63 (2001) 224106.
- [40]. A.F. Voter and S.P. Chen, Accurate Interatomic Potentials for Ni, Al, and Ni₃Al *Mater. Res. Soc. Symp. Proc.* 82 (1987) 175-180.
- [41]. G. Bonny, R.C. Pasianot, N. Castin, and L. Malerba, Ternary Fe-Cu-Ni many-body potential to model reactor pressure vessel steels: First validation by simulated thermal annealing, *Phil. Mag.* 89 (2009) 3531-3546.
- [42]. J.W. Cahn, Y. Mishin, A. Suzuki, Coupling grain boundary motion to shear deformation, *Acta Mater.* 54 (2006) 4953-4975.
- [43]. M. Daw, S.M. Foiles, M.I. Baskes, The embedded-atom method: a review of theory and applications, *Mater. Sci. Rep.* 9 (1993) 251-310.
- [44]. N.Q. Vo, R.S. Averback, Y. Ashkenazy, P. Bellon, J. Wang, Forced chemical mixing at Cu-Nb interfaces under severe plastic deformation, *J. Mater. Res.* 27 (2012) 1621-1630.

- [45]. J.P. Hirth, R.C. Pond, R.G. Hoagland, X.Y. Liu, J. Wang, Interface Defects, Reference Spaces and the Frank-Bilby Equation, *Prog. Mater. Sci.* 58 (2013) 749-823.
- [46]. J. Wang, R.G. Hoagland, A. Misra, Phase transition and dislocation nucleation in Cu–Nb layered composites during physical vapor deposition, *J. Mater. Res.* 23 (2008) 1009-1014.
- [47]. C.B. Carter, The Influence of Jogs on the Extension of Dislocation Nodes, *Phil. Mag. A* 41 (1980) 619-635.
- [48]. S. Sarkar, J. Li, W.T. Cox, E. Bitzek, T.J. Lenosky, Y. Wang, Finding activation pathway of coupled displacive-diffusional defect processes in atomistics: Dislocation climb in fcc copper, *Phys. Rev. B* 86 (2012) 014115.
- [49]. M.J. Demkowicz, R.G. Hoagland, J.P. Hirth, Interface Structure and Radiation Damage Resistance in Cu-Nb Multilayer Nanocomposites, *Phys. Rev. Lett.* 100 (2008) 136102.
- [50]. J. Wang, R.G. Hoagland, A. Misra, Room-temperature dislocation climb in metallic interfaces, *Appl. Phys. Lett.* 94 (2009) 131910.
- [51]. S. Dai, Y. Xiang, D.J. Srolovitz, Atomistic, generalized Peierls-Nabarro, and analytical models for (111) twist boundaries in Al, Cu and Ni for all twist angles, *Acta Mater.* 69 (2014) 162-174.
- [52]. F.Z. Dai, W.Z. Zhang, An automatic and simple method for specifying dislocation features in atomistic simulations, *Comp. Phys. Comm.* 188 (2015) 103-109.
- [53]. S. Huang, J. Wang, C. Zhou, Effect of plastic incompatibility on the strain hardening behavior of Al-TiN nanolayered composites, *Mater. Sci. Eng. A* 636 (2015) 430-433.
- [54]. S. Dai, Y. Xiang, D.J. Srolovitz, Structure and energy of (111) low angle twist boundaries in Al, Cu and Ni, *Acta Mater.* 61 (2013) 1327-1337.
- [55]. M.H. Loretto, Intrinsic and extrinsic nodes in a gold-tin alloy, *Phil. Mag.* 10 (1964) 467-475.
- [56]. J. P. Hirth and J. Lothe, *Theory of Dislocations*, Krieger Pub Co; 2nd edition, 1992.
- [57]. B. Liu, D. Raabe, P. Eisenlohr, F. Roters, A. Arsenlis, G. Hommes, Dislocation interactions and low-angle grain boundary strengthening, *Acta Mater.* 59 (2011) 7125–7134.
- [58]. S.M.A. Khan, H.M. Zbib, D.A. Hughes, Modeling Planar Dislocation Boundaries Using a Multi-Scale Approach, *Int. J. Plast.* 20 (2004) 1059-1092.
- [59]. C.Z. Zhou, S. Biner, R. LeSar, Simulations of the Effect of Surface Coatings on Plasticity at Small Scales, *Scripta Mater.* 63 (2010) 1096-1099.
- [60]. Z. Wang, N. Ghoniem, S. Swaminarayan, R. LeSar, A parallel algorithm for 3D dislocation dynamics, *J. Comp. Phys.* 219 (2006) 608–621.

Table 1. The various EVs in the different regions within the interface.

Node Types			Node (maximum)	Node (integration)	Coherent region	Dislocation line
Volume Smeared	I.	Cu	0.158	17.851	-0.028	0.025
		<i>Ni</i>	-0.069	-13.798	0.022	-0.019
	II.	Cu	0.142	15.503	-0.025	0.009
		<i>Ni</i>	-0.070	-13.732	0.021	-0.009
Volume Condensed	III.(a)	Cu	0.680	18.080	-0.028	0.036
		<i>Ni</i>	-0.071	-15.339	0.024	-0.029
	III.(b)	Cu	0.299	17.084	-0.027	0.023
		<i>Ni</i>	-0.050	-14.460	0.021	-0.019
	III.(c)	Cu	0.336	18.928	-0.032	0.023
		<i>Ni</i>	-0.046	-14.465	0.022	-0.018
	IV.	Cu	0.658	17.676	-0.064	0.041
		<i>Ni</i>	-0.075	-16.325	0.025	-0.033

Table 2. List of all possible lattice dislocations that can be nucleated at various node structures under tensile and compressive loading conditions. We listed line senses (ξ), Burgers vectors ($\mathbf{b}$), slip planes (p), Schmid factor (S), the dot product between the Burgers vectors of the interface and lattice dislocations, and whether the nucleation of the lattice dislocation happened.

Node Structure	Interfacial Dislocation		Lattice Dislocation					$\mathbf{b}_{ID} \cdot \mathbf{b}_{LD}$	Nucleation? (Y/N)
	ξ_{ID}	$\mathbf{b}_{ID}$	ξ_{LD}	$\mathbf{b}_{LD}$	p	S	ξ_{ID}		
Volume condensed-Triangular (Figure 7)	CB	AB	CB	$\alpha\mathbf{B}$	(α)	$\alpha\mathbf{B}$	0.157	0.167	Y
	CB	AB	CB	$\alpha\mathbf{C}$	(α)	$\alpha\mathbf{C}$	0.157	-0.083	N
	CB	AB	CB	$\alpha\mathbf{D}$	(α)	$\alpha\mathbf{D}$	-0.314	-0.083	N
	AC	CB	AC	$\beta\mathbf{C}$	(β)	$\beta\mathbf{C}$	0.157	0.167	Y
	AC	CB	AC	$\beta\mathbf{A}$	(β)	$\beta\mathbf{A}$	0.157	-0.083	N
	AC	CB	AC	$\beta\mathbf{D}$	(β)	$\beta\mathbf{D}$	-0.314	-0.083	N
	BA	CA	BA	$\gamma\mathbf{A}$	(γ)	$\gamma\mathbf{A}$	0.157	0.167	Y
	BA	CA	BA	$\gamma\mathbf{B}$	(γ)	$\gamma\mathbf{B}$	0.157	-0.083	N
	BA	CA	BA	$\gamma\mathbf{D}$	(γ)	$\gamma\mathbf{D}$	-0.314	-0.083	N
Volume condensed-Hexagonal (Fig. 8)	BC	CA	BC	$\mathbf{B}\alpha$	(α)	$\alpha\mathbf{B}$	0.157	-0.083	N
	BC	CA	BC	$\mathbf{C}\alpha$	(α)	$\alpha\mathbf{C}$	0.157	0.167	Y
	BC	CA	BC	$\mathbf{D}\alpha$	(α)	$\alpha\mathbf{D}$	-0.314	-0.083	N
	CA	AB	CA	$\mathbf{C}\beta$	(β)	$\beta\mathbf{C}$	0.157	-0.083	N
	CA	AB	CA	$\mathbf{A}\beta$	(β)	$\beta\mathbf{A}$	0.157	0.167	Y
	CA	AB	CA	$\mathbf{D}\beta$	(β)	$\beta\mathbf{D}$	-0.314	-0.083	N
	AB	BC	AB	$\mathbf{A}\gamma$	(γ)	$\gamma\mathbf{A}$	0.157	-0.083	N
	AB	BC	AB	$\mathbf{B}\gamma$	(γ)	$\gamma\mathbf{B}$	0.157	0.167	Y
	AB	BC	AB	$\mathbf{D}\gamma$	(γ)	$\gamma\mathbf{D}$	-0.314	-0.083	N

Table 3. List of all possible lattice dislocations that can be nucleated at various node structures under compressive loading condition. The same information as in Table 2 is listed.

Node Structure	Interface Dislocation		Lattice Dislocation					$\mathbf{b}_{ID} \cdot \mathbf{b}_{LD}$	Activated? (Y/N)
	ξ_{ID}	$\mathbf{b}_{ID}$	ξ_{LD}	$\mathbf{b}_{LD}$	p	S	ξ_{ID}		
Volume smeared-straight (Fig.10)	CB	A δ	CB	D α	(α)	αD	0.314	0.056	Y
	CB	A δ	CB	B α	(α)	αB	-0.157	-0.028	N
	CB	A δ	CB	C α	(α)	αC	-0.157	-0.028	N
	BC	δA	BC	αD	(α)	αD	0.314	0.056	Y
	BC	δA	BC	αB	(α)	αB	-0.157	-0.028	N
	BC	δA	BC	αC	(α)	αC	-0.157	-0.028	N
	AC	B δ	AC	D β	(β)	βD	0.314	0.056	Y
	AC	B δ	AC	A β	(β)	βA	-0.157	-0.028	N
	AC	B δ	AC	C β	(β)	βC	-0.157	-0.028	N
	CA	δB	CA	βD	(β)	βD	0.314	0.056	Y
	CA	δB	CA	βA	(β)	βA	-0.157	-0.028	N
	CA	δB	CA	βC	(β)	βC	-0.157	-0.028	N
	BA	C δ	BA	D γ	(γ)	γD	0.314	0.056	Y
	BA	C δ	BA	A γ	(γ)	γA	-0.157	-0.028	N
	BA	C δ	BA	B γ	(γ)	γB	-0.157	-0.028	N
	AB	δC	AB	γD	(γ)	γD	0.314	0.056	Y
	AB	δC	AB	γA	(γ)	γA	-0.157	-0.028	N
	AB	δC	AB	γB	(γ)	γB	-0.157	-0.028	N

Figures Captions:

Figure 1. (a) Geometrical feature of FCC (111) interface, showing HESF, ISF, and FCC regions and the corresponding lattice sites that are defined according to geometry analysis. (b) Atomistic structure of the relaxed Cu-Ni interface showing curved dislocation lines, nodes, and two regions ISF and FCC according to geometry analysis. The red regions indicate misfit dislocation lines and nodes.

Figure 2. Illustration of the analysis of excess volume. (a) A triangular mesh is constructed upon atoms positions on a {111} plane using Delaunay triangulation algorithm. (b) For a {111} plane in a perfect crystal, the area occupied by a triangle (A_{bulk}) and an atom (A_{atom}) can be calculated using a simple honeycomb model where $b_{\text{perfect}} = \frac{\sqrt{2}}{2}a$.

Figure 3. (a) Dislocation structure of a volume-smeared node with spiral dislocation pattern (Structure I). The (δ) face of the Thompson's tetrahedron is also given for reference. (b) Atomic structure of the Cu-Ni interface showing the coherent regions (blue) of the interfaces separated by the dislocation lines and intersections (red). (c) and (d) The normalized excess volume distributions for the Cu and Ni sides of the interface, respectively. Darker color represents the lower excess volume, while lighter color represents the higher excess volume. The solid black lines separate the regions with negative excess volume from the regions with positive excess volume.

Figure 4. (a) Dislocation structure of a volume-smeared node with straight dislocation pattern (Structure II). (b) Atomic structure of the Cu-Ni interface showing the wider core at the node and the misfit dislocations compared to Structure I in Fig. 1b. (c) and (d) The excess volume contour plots of the Cu and Ni sides of the interface, respectively.

Figure 5. Excess volume and dislocation structures at the volume-condensed node with “constricted” triangular dislocation pattern (Structure III(a)). (a) The excess volume contour plots for Cu side and (b) the excess volume contour plots for Ni side. (c) The dislocation structures at the node. The condensed excess volume shown in (a) can be treated as the result of the close spacing of the three jogs (green triangle). The node structure involves two sets of interface dislocations on the two adjacent slip planes, the left shows dislocation structure on the interface (Ni1-Cu1) plane, the middle green triangle shows the dislocation in the Cu1-Cu2 plane. The right shows the projection of

the two interface dislocations. In the projected view, the area enclosed by the green triangle is an extrinsic stacking fault (ESF). Green dots represent the jogs that connect two sets of interface dislocations.

Figure 6. Excess volume and dislocation structures at the volume-condensed node with “expanded” triangular dislocation pattern (Structure III(b)) which is created by the absorption of one Cu interstitial. (a) The excess volume contour plots for Cu side and (b) the excess volume contour plots for Ni side. (c) The detailed dislocation structure at the node. The node structure involves two sets of interface dislocations on the two adjacent slip planes, the left shows dislocation structure on the interface (Ni1-Cu1) plane, the middle green triangle shows the dislocation in the Cu1-Cu2 plane. The right shows the projection of the two interface dislocations. In the projected view, the area enclosed by the green triangle is an extrinsic stacking fault (ESF). Green dots represent the jogs that connect two sets of interface dislocations.

Figure 7. Excess volume and dislocation structures at the volume-condensed node with “expanded” triangular dislocation pattern, i.e. Structure III(c) is created by mechanical perturbation. (a) The excess volume contour plots for Cu side and (b) the excess volume contour plots for Ni side. (c) The detailed dislocation structure at the node. The node structure involves two sets of interface dislocations on the two adjacent slip planes, the left shows dislocation structure on the interface (Ni1-Cu1) plane, the middle green triangle shows the dislocation in the Cu1-Cu2 plane. The right shows the projection of the two interface dislocations. In the projected view, the area enclosed by the green triangle is an extrinsic stacking fault (ESF). Green dots represent the jogs that connect two sets of interface dislocations.

Figure 8. Excess volume and dislocation structures at the volume-condensed node with hexagonal dislocation pattern (i.e. Structure IV). (a) The excess volume contour plots for the Cu side and (b) the excess volume contour plots for the Ni side. (c) The detailed dislocation structure at the node. The node structure involves two sets of interface dislocations on the two adjacent slip planes and formed from the triangular node structure after a series of dislocation reactions. On the Ni1-Cu1 plane, six segmental dislocations (three partial, three perfect) enclose a hexagonal area. On the Cu1-Cu2 plane, three segments of partial dislocations also form the same hexagonal shape. The two hexagons

on the two adjacent planes form 6 double-core segmental partial dislocations. The perfect-partial double core dislocations ($A\delta$, $B\delta$ and $C\delta$ in the projected view) correspond to the three concentrations of excess volume in (a). Green dots represent the jogs that connect two sets of interface dislocations.

Figure 9. Nucleation of lattice dislocations from Structure III. (a) Atomic structure and (b) a schematic illustration of (a). The dislocations are characterized using disregistry analysis. (c) & (d) Atomic structure of the Ni side of the interface in the vicinity of the node before and during nucleation, respectively. (e) and (f) The contour plot of excess volume of the Cu side of the interface before and after the nucleation.

Figure 10. Nucleation of lattice dislocations from Structure IV. (a) Illustration of dislocation reaction and nucleation, (b) atomic structure and (c) a schematic illustration of (b). The dislocations are characterized using disregistry analysis. (d) & (e) The contour plot of excess volume of the Cu side of the interface before and after the nucleation.

Figure 11. Nucleation of lattice dislocations from Structure II. (a) Dislocations nucleate near the node from the straight partial segments (marked in red) that are parallel to the traces of slip planes. (b) Atomic configuration of the nucleated dislocation structure. (c) Illustration of the nucleated dislocation structure. (d) After nucleation, the dislocation loops propagate and react with the neighboring loops. Three stair-rod dislocations form as a result (dark red straight lines). This is the illustration of the dislocation structure in (b). (e) The contour plot of excess volume of the Cu side of the interface after the nucleation.

Figure 1. (a) Geometrical feature of FCC (111) interface, showing HESF, ISF, and FCC regions and the corresponding lattice sites that are defined according to geometry analysis. (b) Atomistic structure of the relaxed Cu-Ni interface showing curved dislocation lines, nodes, and two regions ISF and FCC according to geometry analysis. The red regions indicate misfit dislocation lines and nodes.

Figure 2. Illustration of the analysis of excess volume. (a) A triangular mesh is constructed upon atoms positions on a {111} plane using Delaunay triangulation algorithm. (b) For a {111} plane in a perfect crystal, the area occupied by a triangle (A_{bulk}) and an atom (A_{atom}) can be calculated using a simple honeycomb model where $b_{perfect} = \frac{\sqrt{2}}{2}a$.

Figure 3. (a) Dislocation structure of a volume-smeared node with spiral dislocation pattern (Structure I). The (δ) face of the Thompson's tetrahedron is also given for reference. (b) Atomic structure of the Cu-Ni interface showing the coherent regions (blue) of the interfaces separated by the dislocation lines and intersections (red). (c) and (d) The normalized excess volume distributions for the Cu and Ni sides of the interface, respectively. Darker color represents the lower excess volume, while lighter color represents the higher excess volume. The solid black lines separate the regions with negative excess volume from the regions with positive excess volume.

Figure 4. (a) Dislocation structure of a volume-smeared node with straight dislocation pattern (Structure II). (b) Atomic structure of the Cu-Ni interface showing the wider core at the node and the misfit dislocations compared to Structure I in Fig. 1b. (c) and (d) The excess volume contour plots of the Cu and Ni sides of the interface, respectively.

Figure 5. Excess volume and dislocation structures at the volume-condensed node with “constricted” triangular dislocation pattern (Structure III(a)). (a) The excess volume contour plots for Cu side and (b) the excess volume contour plots for Ni side. (c) The dislocation structures at the node. The condensed excess volume shown in (a) can be treated as the result of the close spacing of the three jogs (green triangle). The node structure involves two sets of interface dislocations on the two adjacent slip planes, the left shows dislocation structure on the interface (Ni1-Cu1) plane, the middle green triangle shows the dislocation in the Cu1-Cu2 plane. The right shows the projection of the two interface dislocations. In the projected view, the area enclosed by the green triangle is an extrinsic stacking fault (ESF). Green dots represent the jogs that connect two sets of interface dislocations.

Figure 6. Excess volume and dislocation structures at the volume-condensed node with “expanded” triangular dislocation pattern (Structure III(b)) which is created by the absorption of one Cu interstitial. (a) The excess volume contour plots for Cu side and (b) the excess volume contour plots for Ni side. (c) The detailed dislocation structure at the node. The node structure involves two sets of interface dislocations on the two adjacent slip planes, the left shows dislocation structure on the interface (Ni1-Cu1) plane, the middle green triangle shows the dislocation in the Cu1-Cu2 plane. The right shows the projection of the two interface dislocations. In the projected view, the area enclosed by the green triangle is an extrinsic stacking fault (ESF). Green dots represent the jogs that connect two sets of interface dislocations.

Figure 7. Excess volume and dislocation structures at the volume-condensed node with “expanded” triangular dislocation pattern, i.e. Structure III(c) is created by mechanical perturbation. (a) The excess volume contour plots for Cu side and (b) the excess volume contour plots for Ni side. (c) The detailed dislocation structure at the node. The node structure involves two sets of interface dislocations on the two adjacent slip planes, the left shows dislocation structure on the interface (Ni1-Cu1) plane, the middle green triangle shows the dislocation in the Cu1-Cu2 plane. The right shows the projection of the two interface dislocations. In the projected view, the area enclosed by the green triangle is an extrinsic stacking fault (ESF). Green dots represent the jogs that connect two sets of interface dislocations.

Figure 8. Excess volume and dislocation structures at the volume-condensed node with hexagonal dislocation pattern (Structure IV). (a) The excess volume contour plots for Cu side and (b) the excess volume contour plots for Ni side. (c) The detailed dislocation structure at the node. The node structure involves two sets of interface dislocations on the two adjacent slip planes and formed from the triangular node structure after a series of dislocation reactions. On the Ni1-Cu1 plane, six segmental dislocations (three partial, three perfect) enclose a hexagonal area. On the Cu1-Cu2 plane, three segments of partial dislocations also form the same hexagonal shape. The two hexagons on the two adjacent planes form 6 double-core segmental partial dislocations. The perfect-partial double core dislocations ($A\delta$, $B\delta$ and $C\delta$ in the projected view) correspond to the three concentrations of excess volume in (a). Green dots represent the jogs that connect two sets of interface dislocations.

Figure 9. Nucleation of lattice dislocations from Structure III. (a) Atomic structure and (b) a schematic illustration of (a). The dislocations are characterized using disregistry analysis. (c) & (d) Atomic structure of the Ni side of the interface in the vicinity of the node before and during nucleation, respectively. (e) and (f) The contour plot of excess volume of the Cu side of the interface before and after the nucleation.

Figure 10. Nucleation of lattice dislocations from Structure IV. (a) Illustration of dislocation reaction and nucleation, (b) atomic structure and (c) a schematic illustration of (b). The dislocations are characterized using disregistry analysis. (d) and (e) The contour plot of excess volume of the Cu side of the interface before and after the nucleation.

Figure 11. Nucleation of lattice dislocations from Structure II. (a) Dislocations nucleate near the node from the straight partial segments (marked in red) that are parallel to the traces of slip planes. (b) Atomic configuration of the nucleated dislocation structure. (c) Illustration of the nucleated dislocation structure. (d) After nucleation, the dislocation loops propagate and react with the neighboring loops. Three stair-rod dislocations form as a result (dark red straight lines). This is the illustration of the dislocation structure in (b). (e) The contour plot of excess volume of the Cu side of the interface after the nucleation.