Structure, shear resistance, and interaction with point defects of interfaces in Cu-Nb nanocomposites synthesized by severe plastic deformation

M. J. Demkowicz[1, *], L. Thilly[2, †]

[1]Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139
[2]Pprime Institute, Department of Materials Physics and Mechanics, CNRS-University of Poitiers-ENSMA, Poitiers, France

Abstract

We use atomistic modeling to investigate the shear resistance and interaction with point defects of a Cu-Nb interface found in nanocomposites synthesized by severe plastic deformation. The shear resistance of this interface is highly anisotropic: in one direction shearing occurs at stresses below 1200MPa while in the other it does not occur at all. The binding energy of vacancies, interstitials, and He impurities to this interface depends sensitively on the binding location, but there is no point defect delocalization nor does this interface contain any constitutional defects. These behaviors are markedly dissimilar from a different Cu-Nb interface found in magnetron sputtered composites. The dissimilarities may, however, be explained by quantitative differences in the detailed structure of these two interfaces.

* Corresponding author: demkowicz@mit.edu
617-324-6563
MIT, room 4-142
77 Massachusetts Ave.
Cambridge, MA 02139
† ludovic.thilly@univ-poitiers.fr

I. Background

Interfaces often play a determining role for the properties of polycrystalline solids [1]. They are especially important in materials with nanometer-scale microstructural dimensions, since a sizeable fraction of atoms in such materials resides at or near interfaces. Much recent research on novel structural materials aims to exploit the influence of interfaces [2], e.g. to improve wear resistance of electrodeposited nanostructured alloys [3-5] or to heal radiation damage in magnetron sputtered nanocomposites [6-9]. Due to improvements in characterization and modeling techniques, interfaces may now be studied with unprecedented detail and precision [10]. The full three-dimensional atomic structure of interfaces may be investigated and its effect on properties assessed, opening opportunities for developing quantitative structure-property relations for specific interfaces, similar to what has been done for bulk solids.

In this study, we use atomistic modeling to study one specific heterophase interface between face-centered cubic copper (fcc Cu) and body-centered cubic niobium (bcc Nb) found in nanocomposites formed by two different severe plastic deformation (SPD) techniques: accumulative drawing and bundling (ADB) [11, 12] and accumulated roll bonding (ARB) [13, 14]. We then compare our results to prior work on another type of Cu-Nb interface found in magnetron sputtered composites [6, 9, 15-19]. Although these two interfaces have many *qualitative* structural features in common, they exhibit marked dissimilarities in certain properties. These dissimilarities, however, may be explained based on *quantitative* differences in interface structure, motivating the need for improved structure-property descriptions for interfaces in general.

In ADB, an initial billet composed of an oxygen-free high-conductivity (OFHC) Cu jacket containing a Nb core is subjected to repeated cycles of hot extrusion, wire drawing, and bundling and is thereby transformed into a Cu wire containing several millions of Nb nanofilaments [11, 12, 20]. Extreme total strains typically larger than 20 are imposed on both the Cu and Nb phases and, as a result, the Cu matrix and the Nb filaments become nanocrystalline with elongated grains in the wire axis direction and cross-section sizes in the 200-400nm and 50-100nm ranges, respectively [21].

Moreover, both components are strongly textured after ADB: X-ray diffraction evidenced a predominant macroscopic <111> axial texture of the Cu matrix (along with a remnant <100> component associated with dynamic recrystallization in the thicker parts of the Cu matrix) and a very strong <110> axial texture for the Nb nanofilaments. In other words, after repeated activation of dislocation slip, the Cu and Nb grains are oriented such that their respective $\{111\}_{Cu}$ and $\{110\}_{Nb}$ planes (the densest planes, in both components) are parallel to each other and normal to the drawing direction.

The atomic arrangement of Cu-Nb interfaces in the ADB nanocomposites was studied using high resolution transmission electron microscopy (HRTEM). Although Cu and Nb are merely in mechanical contact in the initial billet, they are remarkably well bonded at the atomic scale after SPD, as shown in Fig. 1.a). Because of the above-mentioned textures, $\{111\}_{Cu}$ and $\{110\}_{Nb}$ planes are nearly parallel at most of the Cu-Nb interfaces. A misorientation of a few degrees (4.5° in the case of Fig. 1) between them, however, has been repeatedly observed [11, 12].

The image filtered micrograph in Fig. 1.b) shows that the Cu-Nb interfaces are semicoherent with misfit dislocations in Cu every eight or nine $\{111\}_{Cu}$ atomic planes, which compensate for the ~10% misfit between $d(\{111\}_{Cu})$=2.08Å and $d(\{110\}_{Nb})$=2.33Å [11, 12]. The formation of such clean and specifically oriented Cu-Nb interfaces has been attributed to the so-called "single dislocation" mechanism associated with whisker-like deformation of the fine Cu matrix and Nb nanofilaments [12]. Similar Cu-Nb interfaces have been observed in other studies on ADB nanocomposites, the interface planes being often observed as $\{112\}_{fcc}||\{112\}_{bcc}$ [11, 12, 22-24].

Interfaces with the same orientation relation and interface plane as described above have also been found in multilayer Cu-Nb composites fabricated by ARB. In this process, Cu and Nb plates are repeatedly stacked and rolled, once again reducing their microstructural dimensions to nanometer levels [13]. With successive cycles, the composite develops a texture in the rolling direction similar to that found in the wire direction in ADB composites, namely $\{111\}_{Cu}$ and $\{110\}_{Nb}$ planes are parallel to each other and normal to the rolling direction. TEM investigations have shown that the crystallography and atomic structure of the interfaces found in ARB composites after multiple rolling cycles is the same as that in Fig. 1 [14].

The investigation we present here focuses on relating the structure of the interface described above to its shear resistance and its interaction with point defects. Shear resistance has been linked to the ability of interfaces to trap glide dislocations [25-29]. By impeding dislocation transmission between neighboring crystals, low shear resistance interfaces may strengthen composite materials to near-theoretical levels [27-34]. Interactions with point defects determine how an interface influences damage sustained under irradiation [7]. By trapping and accelerating recombination of vacancies and interstitials, interfaces may mitigate radiation-induced degradation phenomena such as hardening and swelling [8, 27, 35, 36]. Interfaces with high free volume have been shown to trap implanted He impurities, thereby delaying bubble formation [36-38].

II. Construction of an interface model

We begin our study by building an atomic model that describes the structure and bonding at the interface of interest. Cu and Nb have high positive heats of mixing, do not form compounds, and exhibit limited solid solubility [39]. The Cu-Nb system can

therefore be reliably modeled using a previously developed embedded atom method (EAM) classical potential [40, 41]. Some of the simulations described here were performed with the LAMMPS code [42] and others with a code belonging to MJD.

The interface of interest here forms along $\{112\}_{fcc}||\{112\}_{bcc}$ planes and the adjacent Cu and Nb crystals are oriented with respect to each other within <5° of the Kurdjumov-Sachs (KS) [43] relation:

$$\begin{aligned} &\langle 111\rangle_{fcc}||\langle 110\rangle_{bcc} \\ &\langle 110\rangle_{fcc}||\langle 111\rangle_{bcc}. \end{aligned} \qquad 1$$

Interfaces with this crystallography may be constructed by joining fcc Cu and bcc Nb crystalline layers as illustrated in Fig. 2. The layers are periodic parallel to the interface, terminate with free surfaces in the direction normal to it, and are at least 4nm thick to minimize the influence of free surfaces on the interface. The interface is not strictly periodic when stress free, so strains had to be applied to one or both of the neighboring layers to impose periodic boundaries. We minimized these "periodicity strains" by judiciously choosing our system size. No strain component larger than 0.6% was required in any of the bilayer models.

In addition to the "macroscopic" crystallographic variables represented by the orientation relation and interface plane, we considered two types of microscopic variables: translations of the adjoining Cu and Nb layers parallel to the interface as well as variations in the number of interface Cu and Nb atoms per unit area. We did not investigate the effect of intermixing because of the negligible mutual solid solubility of Cu and Nb [39].

To investigate relative translations, we constrained atomic displacements so that the adjoining Cu and Nb layers could only displace as rigid bodies: their constituent atoms were not allowed to displace independently. For every desired relative translation parallel to the interface plane, the displacement normal to the interface was relaxed to its minimum energy value. As in previous studies [27, 29], the resulting dependence of interface energy on relative translations may be represented as a γ-surface [44].

To compute interface energies, we break up the total potential energy of the bilayer, E_{bl}, into contributions from the interface, free surfaces, and the cohesive energies of the Cu and Nb atoms:

$$E_{bl} = \gamma_i^{Cu-Nb} A + \gamma_{fs}^{Cu} A + \gamma_{fs}^{Nb} A + E_{coh}^{Cu} N^{Cu} + E_{coh}^{Nb} N^{Nb}.$$

Here, γ_i^{Cu-Nb} is the energy (per unit area) of the Cu-Nb interface, γ_{fs}^{Cu} and γ_{fs}^{Nb} are the energies of the Cu and Nb free surfaces, respectively, and A is the interface area (by

construction, it is equal to the free surface areas). E_{coh}^{Cu} and E_{coh}^{Nb} are the cohesive energies per atom of Cu and Nb, respectively, while N^{Cu} and N^{Nb} are the total numbers of Cu and Nb atoms in the system. The interface energy may therefore be computed as

$$\gamma_i^{Cu-Nb} = \frac{1}{A}\left(E_{bl} - E_{coh}^{Cu}N^{Cu} - E_{coh}^{Nb}N^{Nb}\right) - \gamma_{fs}^{Cu} - \gamma_{fs}^{Nb}.$$

The cohesive energies E_{coh}^{Cu} and E_{coh}^{Nb} are computed from perfect crystalline fcc Cu and bcc Nb while the free surface energies γ_{fs}^{Cu} and γ_{fs}^{Nb} are found from Cu and Nb sheets with free surfaces identical to those in the Cu-Nb bilayer.

The γ-surface was found to be flat along x-direction (<110>$_{Cu}$, see Fig. 2) to within 0.2mJ/m^2. Along the z-direction (<111>$_{Cu}$) it is sinusoidal with a peak-to-trough energy difference of ~22mJ/m^2 and period of ~1.5Å. Thus, this interface has no isolated metastable minima under relative rigid body translations of the neighboring layers, but the global minimum is degenerate with respect to translations along <110>$_{Cu}$.

Next, we relaxed all atomic positions independently at zero temperature using conjugate gradient energy minimization. A structure obtained by relaxing starting from a γ-surface minimum has an energy over 370mJ/m^2 lower than that obtained by relaxing from a γ-surface maximum. When this low energy interface is further annealed by molecular dynamics for ~10ns at 800K and quenched back to zero temperature, its energy is further reduced by over 125mJ/m^2, giving a final interface energy of about 820mJ/m^2.

We gaged the sensitivity of interface energy to changes in its local density and composition by computing the formation energies of Cu and Nb vacancies and interstitials over a wide range of locations within the interface (see section V). Vacancy formation energies at atoms of type x (x=Cu, Nb), ΔE_{vx}^f, were computed as

$$\Delta E_{vx}^f = \left(E_{bl}^{final} + E_{coh}^x\right) - E_{bl}^{initial},$$

where $E_{bl}^{initial}$ is the bilayer potential energy before creation of the vacancy, E_{bl}^{final} is its energy with the vacancy, and E_{coh}^x is the cohesive energy of atom x. Similarly, formation energies of interstitial atoms of type x, ΔE_{ix}^f, were computed as

$$\Delta E_{ix}^f = E_{bl}^{final} - \left(E_{bl}^{initial} + E_{coh}^x\right).$$

If a negative vacancy or interstitial formation energy is found, then the introduction of that point defect lowers the energy of the interface. To find the ground state interface configuration, vacancies and interstitials must be iteratively added until no negative formation energy sites remain. Using this approach or related ones, the ground states of some interfaces have been shown to have local densities and compositions markedly different from the neighboring crystals [8, 37, 45, 46]. In the interface studied here, however, no negative vacancy or interstitial formation energy sites were found.

We consider the model constructed as described above to be representative of the lowest energy interface configuration. All of our calculations, however, were conducted at zero temperature. The minimum *free* energy interface structure at elevated temperature might differ from the one we obtained. Studies conducted on grain boundaries indicate that high temperature structural transitions of this sort do indeed occur, though typically at homologous temperatures greater than 0.5 (~680K for Cu) [47, 48]. Our model is therefore likely representative of the lowest free energy interface structure over a wide range of sufficiently low temperatures, including the ones at which the characterizations described in section I were conducted (i.e. room temperature).

III. Interface structure

III.a Misfit dislocation configuration

Figures 3.a) and 3.b) respectively show edge-on and plan views of the relaxed interface. Inspection of Fig. 3.a) suggests that this interface contains at least two different sets of parallel misfit dislocations aligned with the x-direction: some with compact, undissociated cores [labeled as "1" in Fig. 3.a)] and others that dissociate into Shockley partials [labeled "2" in Fig. 3.a)].

A primer on the classical theory of misfit dislocations may be found in reference [1]. Following previous studies [27, 49], we characterize misfit dislocation content quantitatively by computing the disregistry between the Cu and Nb side of the interface. Disregistry is the difference between the relative positions of an interface Cu and Nb atom in the relaxed interface and that same pair of atoms in a coherent reference structure:

$$\vec{D} = \Delta\vec{r}^{\,coherent}_{Cu_i - Nb_j} - \Delta\vec{r}^{\,relaxed}_{Cu_i - Nb_j}. \qquad 2$$

We choose a reference structure where the Nb side has been strained to coherency with Cu (through the Bain transformation) and compute the disregistry $\vec{D}$ as a function of position in the interface plane, i.e. as a function of the x- and z-coordinates. Disregistry is therefore a 2-vector-dependent 3-vector field. It

undergoes rapid variation at dislocation cores by a total amount equal to the Burgers vector and is flat otherwise.

The contribution to disregistry of any dislocation whose line direction is parallel to the x-axis does not depend on x. Thus, if disregistry plotted as a function of z alone collapses onto a single curve, this demonstrates that any dislocations contributing to the disregistry are aligned with the x-axis. Conversely, any dislocation not parallel to x will produce an x-dependent disregistry that cannot be plotted as a function of z alone.

Figure 4 shows that all the data for the y and z disregistry components, in Fig. 4.b) and 4.c), indeed collapse onto a single curve when plotted as a function of z. Thus, all misfit dislocations with Burgers vectors containing y- and z-components lie along the x-direction. By contrast, the x-disregistry in Fig. 4.a) does not collapse onto a single curve when plotted as a function of z, demonstrating that there are misfit dislocations in the interface with Burgers vectors lying entirely along the x-axis, but line directions not along the x-axis.

Analyzing Fig. 4.b) and 4.c), we can unambiguously confirm the presence of two sets of misfit dislocations and measure their spacings as well as y and z Burgers vector components. In Fig. 4.b), dislocation cores appear as sudden steps in disregistry. There are two sets of such steps, labeled 1 and 2, whose locations correspond to the dislocation cores identified with the same labels in Fig. 3.a). These two sets of steps have the same spacings, but different step heights. The size of each step corresponds to the Burgers vector y-component of a dislocation.

By contrast, Fig. 4.c) contains only one set of steps. These steps are not as sharp as in Fig. 4.b), giving evidence of dislocation core spreading in the interface plane. They are nevertheless distinct and give rise to an unambiguous Burgers vector z-component. The locations of these steps align with those of the set 1 steps in Fig. 4.b), suggesting that both belong to the same interface misfit dislocations.

Parameters characterizing misfit dislocation sets 1 and 2 obtained from analysis of disregistry are summarized in Table I. The spacing of set 1 misfit dislocations is in excellent agreement with the experimental observations described in section I. Further analysis of the disregistry x-component in Fig. 4.a) did not yield insights concerning its origin. An analytical calculation of interface dislocation content, as described by the Frank-Bilby equation [1, 27, 50], does, however, shed additional light on the interface misfit dislocation structure.

Suppose $\mathbf{F}_{\mathbf{Cu}}^{-1}$ and $\mathbf{F}_{\mathbf{Nb}}^{-1}$ are displacement gradients that describe the deformation that must be applied respectively to the fcc Cu and bcc Nb sides of the interface to obtain a coherent reference structure. Then the Frank-Bilby equation gives the sum of Burgers vectors $\vec{B}$ from dislocations crossing a line $\vec{p}$ in the interface as

$$\vec{B} = \left(\mathbf{F}_{\mathbf{Cu}}^{-1} - \mathbf{F}_{\mathbf{Nb}}^{-1}\right)\vec{p}. \quad 3$$

If the coherent reference state is chosen to be fcc Cu, then $\mathbf{F}_{\mathbf{Cu}} = \mathbf{I}$, where $\mathbf{I}$ is the identity tensor, and $\mathbf{F}_{\mathbf{Nb}}$ describes the stretch and rotation that, when applied to an fcc metal with the lattice parameter of Cu, results in a bcc lattice with the lattice parameter of Nb in the KS orientation relation with respect to the coherent reference state. Then,

$$\vec{B} = \left(\mathbf{I} - \mathbf{F}_{\mathbf{Nb}}^{-1}\right)\vec{p}. \quad 4$$

We may additionally account for the small strains that had to be applied to build the interface model under periodic boundary conditions, as stated in section II. Calling $\mathbf{S}_{\mathbf{Cu}}$ the displacement gradient applied to the fcc Cu side and $\mathbf{S}_{\mathbf{Nb}}$ that applied to the Nb side, we get

$$\vec{B} = \left(\mathbf{S}_{\mathbf{Cu}}^{-1} - \mathbf{F}_{\mathbf{Nb}}^{-1}\mathbf{S}_{Nb}^{-1}\right)\vec{p}. \quad 5$$

The standard analysis method described in [51] may be used to calculate the spacing and line directions of interface misfit dislocations such that they account for the dislocation content described by Eqn. 5. This method requires sets of trial values of the misfit dislocations' Burgers vectors to be chosen. Each set must contain three linearly independent Burgers vectors. In this study, we assumed that the misfit dislocation Burgers vectors are of the $\frac{1}{2}\langle 110\rangle$ type in the reference fcc Cu crystal. Thus, ignoring vector sense, there are six possible Burgers vector directions. The number of combinations of 3 elements out a set of 6 is 20. The number of co-planar, and therefore linearly dependent, groups of three Burgers vectors is equal to the number of faces of the Thompson tetrahedron, i.e. 4. The number of linearly independent combinations of Burgers vectors is therefore 20-4=16, yielding sixteen different calculated misfit dislocation configurations. Of these, only four are consistent with the disregistry data for dislocation sets 1 and 2 given in Table I.

In all four, the Burgers vectors of set 1 and 2 dislocations have an x-component and there is furthermore a third set of misfit dislocations with Burgers vector lying exclusively along the x-direction. The dashed lines in Fig. 3.b) show the predicted line directions of the third set in these four solutions [the direction is identical in two of the solutions, which is why Fig. 3.b) only contains three dashed lines]. In agreement with our analysis of Fig. 4.a), the third set of dislocations does not lie along the x-axis in any of the four solutions.

Of the four possible solutions, we consider the one that predicts the largest spacing between set 3 dislocations as the most likely since it minimizes dislocation line length per unit interface area and therefore may minimize interface energy as well.

The set 3 line direction from this solution is given in Table I and illustrated with the thick dashed line in Fig. 3.b). Table I also gives the set 3 spacing and Burgers vector as well as the x-component of the Burgers vectors of set 1 and 2 dislocations predicted in this solution to the Frank-Bilby equation.

III.b Effect of deviation from pure Kurdjumov-Sachs orientation relation

As described in Section I, TEM investigations have shown that the orientation relation between Cu and Nb at the interface we are studying may deviate from pure Kurdjumov-Sachs (Eqn. 1) by a tilt of a few degrees about the $<110>_{Cu}$ direction in the interface plane. For a tilt angle α, we express this deviation as a rotation matrix $\mathbf{R}(\alpha)$ of the Cu crystal. Using the trial Burgers vectors given in Table I, we investigate the effect of tilt on the interface misfit dislocation configuration by solving the Frank-Bilby equation

$$\vec{B} = \left(\mathbf{R}^{-1}(\alpha) - \mathbf{F}_{\mathbf{Nb}}^{-1}\right)\vec{p}\,. \qquad 6$$

and find that the spacing of the set 2 misfit dislocations varies markedly as a function of α while the distribution of the remaining misfit dislocations is not significantly affected.

At a tilt of $\alpha \approx 7.1°$, this analysis predicts an infinite spacing of the set 2 misfit dislocations. We construct a model of the interface with a tilted Cu crystal to verify this prediction. As before, to impose periodic boundary conditions parallel to the interface plane, a slight strain had to be applied on the crystalline layers. For a maximum strain component magnitude of 1.3%, no set 2 misfit dislocations are found at a tilt of $\alpha \approx 6.7°$ of the Cu crystal. The slight deviation in tilt angle from the predicted value (7.1°) may be attributed to a modification of misfit dislocation spacing arising from the strain that had to be applied to impose periodic boundaries. Since periodicity strains may be reduced in models of larger interface area, the value of α at which no set 2 dislocations are found is expected to approach the analytically computed value of $\sim 7.1°$ in larger simulation cells.

Figure 5 shows the Cu-Nb interface constructed above. As in the case with no tilt applied, the set 1 misfit dislocations are aligned with the x-axis. Their cores are clearly discernible in the edge-on view in Fig. 5.a). Since there are no set 2 misfit dislocations, no Shockley partials are emitted into the Cu layer, unlike in Fig. 3.a). Fig. 5.b) shows that the most likely orientation of set 3 misfit dislocations changes slightly as a result of the applied tilt.

The Cu-Nb interface in Fig. 5 has an energy of about 690 mJ/m^2, i.e. ~130 mJ/m^2 lower than the interface with no tilt applied, shown in Fig. 3. If this difference in energy is attributed to the set 2 misfit dislocations—which are present in the

former, but not in the latter—then every set 2 misfit dislocation contributes an energy of 0.24 nJ/m or 0.15 eV/Å. This energy is in reasonable agreement with the order-of-magnitude estimate of dislocation line energy $\mu b^2/4\pi \approx 0.25$ eV/Å (for μ=80GPa and b=2.5Å) [50] and may account for the deviation from the perfect Kurdjumov-Sachs orientation relation observed in TEM investigations and shown in Fig. 1.a) [11, 12].

IV. Interface shear resistance

Interface shear resistance was investigated at zero temperature under displacement control. Simple shear was imposed along the interface by forcing two slabs of atoms enclosing the free surfaces of the Cu-Nb bilayer to undergo successive increments of rigid body translation parallel to the interface. The atoms that make up the slabs are not allowed to displace independently, but each slab may translate as a rigid body. The positions of all atoms between the slabs are allowed to change independently. The thickness of each slab is twice the cutoff radius of the Cu-Nb EAM potential, isolating the atoms between the slabs from the vacuum outside. Slab displacements were chosen to give 0.1% increments of average strain in the material in-between. After each displacement, the slab coordinates parallel to the interface were held fixed, but translations normal to the interface were allowed.

The system potential energy under these constraints was minimized using the conjugate gradient method. At the end of the relaxation, there remain unbalanced forces acting on atoms in each of the slabs. The resultant of these forces divided by the slab surface area is equal and opposite to the tractions that must be applied to maintain the slabs in their displaced positions. These in turn are equal to the shear stresses acting on the interface. As expected, the tractions on the two slabs are always equal and opposite and the traction component normal to the interface is zero (since the slabs may displace rigidly in that direction during relaxation).

Simulations were performed for twelve different shearing directions parallel to the interface. Both interfaces with and without Shockley partials (SPs) emitted by set 2 misfit dislocations (shown in Fig. 3 and 5, respectively) were investigated. A remarkably consistent picture emerges from these calculations: when the shearing displacements applied across the interface have a component parallel to the x-axis, interface sliding occurs in the x-direction at stress magnitudes $|\sigma_{xy}|$ between 800 to 1200MPa, far below the theoretical shear resistance of either Cu or Nb. By contrast, regardless of the applied displacements, no interface sliding occurs in the z-direction.

Figure 6 shows examples of stress-strain curves obtained in an interface structure with SPs (Fig. 3) for shear displacements of the Cu slab applied along $\hat{l} = \frac{\sqrt{3}}{2}\hat{x} + \frac{1}{2}\hat{z}$ as well as along the opposite direction, $-\hat{l}$. The figure also shows the x- and z-

components of the average displacement discontinuity $\Delta\vec{u} = \vec{u}_{Cu} - \vec{u}_{Nb}$ across the interface for shearing along both directions ($\vec{u}_{Cu}$ and $\vec{u}_{Nb}$ are the displacements of the Cu and Nb interface atomic layers, respectively).

For displacements along $-\hat{l} = -\frac{\sqrt{3}}{2}\hat{x} - \frac{1}{2}\hat{z}$ [Fig. 6.a)], slip along the x-direction initiates at the interface when σ_{xy}≈-1200MPa and continues at a steady rate —evidenced by the constantly decreasing value of Δu_x — while σ_{xy} undergoes low-amplitude variations about -1200MPa. By contrast, Δu_z remains zero through the shearing process, showing that no slip across the interface occurs in the z-direction. σ_{yz} also reaches a steady state, albeit at around -300MPa. At this stress, SPs begin to extend and continue to move away from the interface, as shown in Fig. 7.b), until they impinge on one of the slabs upon which displacements were imposed to shear the system. The downturn in σ_{yz} in the shaded region of Fig. 6.a) is due to this impingement and is therefore not representative of the true shearing response of the interface. The steady-state value of σ_{yz} is easily rationalized as the resolved stress needed to propagate a Shockley partial in Cu if its motion is opposed by the cost of creating a stacking fault: $\gamma_{SF}/b_{SP} \approx 300$MPa, where we have used $\gamma_{SF} = 45$ mJ/m^2 for the intrinsic stacking fault energy in Cu [50] and $b_{SP} = 1.47$ Å for the Burgers vector of a SP in Cu.

For shearing along $\hat{l} = \frac{\sqrt{3}}{2}\hat{x} + \frac{1}{2}\hat{z}$ [Fig. 6.b)], slip also only occurs along the x-direction and never along the z-direction. In this case, however, the applied stress pushes the SPs back into the interface, rather than away from it. The perturbation in the stress-strain and $\Delta\vec{u}$ -strain curves at a strain of 0.045 in Fig. 6.b) is due to the re-absorption of the SPs at the interface when σ_{yz}≈600MPa. Simultaneously, the shear stress σ_{xy} required for interface sliding decreases from ~1000 to ~800MPa, but the interface shearing response is otherwise unchanged. Upon continued shearing, σ_{yz} increases monotonically.

Similar responses to those described above were found for shearing along all other directions parallel to the interface. Whenever the shearing displacement had an x-component, the interface slipped in the x-direction when σ_{xy}≈-1200MPa (for negative x-displacements) or σ_{xy}≈1000MPa (for positive x-displacements). No slip in the z-direction was ever observed regardless of the shearing direction or magnitude of applied stresses. For shearing displacements with a negative z-component, SPs moved away from the interface at σ_{yz}≈-300MPa whereas for positive z-component displacements they were re-absorbed at the interface when σ_{yz}≈600MPa. At critical σ_{yz} values typically between 2000 to 3500MPa, isolated SPs or groups of SPs are emitted from the interface, as illustrated in Fig. 7.c). The number of such defects, their spacing, and the stress at which they are emitted varies from calculation to calculation and likely depends on the detailed microstructure and loading conditions in a real Cu-Nb composite.

The shear response of Cu-Nb interfaces without SPs (Fig. 5) is qualitatively the same as those with SPs: interface slip occurs readily in the x-direction (at $|\sigma_{xy}|$ magnitudes slightly lower than for the interface with SPs) and never in the z-direction. For shearing displacements with a non-zero z-component, $|\sigma_{yz}|$ increases monotonically. For critical $|\sigma_{yz}|$ values between 2000 and 4500MPa, isolated SPs or groups thereof are emitted. As may be expected, however, this interface does not exhibit any of the phenomena associated with the extension or absorption of pre-existing SPs that were described above. For example, there is no perturbation in the stress-strain or $\Delta\vec{u}$ -strain curves, such as the one in Fig. 6.b), for shearing displacements with a positive z-component. The shearing response of Cu-Nb interfaces with and without SPs is summarized in the yield surface in Fig. 7.a).

Following previous studies [27-29], to gain insight into the mechanisms of interface shearing, we analyzed the distribution of disregistry $\vec{D}$ (Eqn. 2) across the Cu-Nb interface as it slipped in the x-direction. Disregistry was computed as described in Section III using the interface at zero strain as a reference state. Figure 8 shows a vector plot of disregistry for increasing magnitudes of $\Delta\vec{u}$ in an interface that contains SPs (Fig. 3). Individual $\vec{D}$ values have a pronounced x-component and negligible z-component, reflecting the fact that no slip occurs across the interface in the z-direction.

The shaded areas in Fig. 8 denote regions with disregistry magnitudes exceeding 1.65Å. Fig. 8.a) shows that the onset of shearing is not uniform across the interface, but rather initiates at sites of lowest shear resistance. As slip continues, the sheared areas extend and eventually coalesce, as shown in Fig. 8.d). The orientation of the sheared areas in Fig. 8.d) corresponds to the most likely direction of set 3 misfit dislocations, predicted in Section III and shown in Fig. 3.b). Furthermore, since their Burgers vectors lie along the x-direction, the glide of successive segments of these dislocations within the interface may lead to a disregistry pattern such as that shown in Fig. 8. The glide of these dislocations may therefore be responsible for the ease of interface slip along the x-direction. Correspondingly, the high interface shear resistance in the z-direction may arise from the lack of misfit dislocations with a z-component in their Burgers vectors that may also glide in the interface plane.

V. Interface interaction with point defects

To assess trapping of point defects at Cu-Nb interfaces, we compared the formation energies of vacancies, interstitials, and He impurities at these interfaces with corresponding formation energies in fcc Cu and bcc Nb. Starting with a given interface structure, vacancies were created by deleting an atom, substitutional impurities by changing the chemical identity of an atom, and interstitials by inserting an atom at a desired location.

Defect structures were relaxed at constant volume by a three-step process: (i) conjugate gradient energy minimization to relax configurations with closely spaced atoms that may arise due to interstitial insertion, (ii) molecular dynamics (MD) annealing at 300K for 10ps to overcome any small barriers that may trap the structure in shallow potential energy minima, and finally (iii) conjugate gradient energy minimization to remove thermal motion from the annealed structure. In computing point defect formation energies, we assumed Cu and Nb chemical potentials equal to their atomic cohesive energies in fcc and bcc crystals, respectively. To find He impurity energies, we used a recently developed Cu-Nb-He potential [52] and assumed zero chemical potential for He.

Figure 9 shows the dependence of vacancy formation energy on distance from an initially point defect-free Cu-Nb interface containing Shockley partials emitted by set 2 misfit dislocations [see Fig. 3.a)]. As expected, sufficiently far from the interface, vacancies have the same formation energies as in perfect crystalline fcc Cu and bcc Nb. Near the interface, however, formation energies are highly variable and depend on the location of vacancies within the interface.

Three trends in vacancy formation energy may be distinguished. At some sites, labeled "A" in Fig. 9, vacancy formation energies are intermediate between those of fcc Cu and bcc Nb and change gradually over five atomic layers as a function of position normal to the interface. Nb vacancies may become trapped at these sites, but Cu vacancies would be repelled from them. At other sites, labeled "B" in Fig. 9, vacancy formation energies are lower than in either fcc Cu or bcc Nb. Such sites are found predominantly on the Cu side of the interface and are traps for both Cu and Nb vacancies. Finally, sites labeled "C" are shallow vacancy traps located at the Shockley partials and associated stacking faults emitted into Cu by set 2 misfit dislocations, as illustrated in Fig. 3.a).

The variation of vacancy formation energies within the Cu and Nb atomic planes that meet at the interface is shown in Fig. 10. Unlike in certain other Cu-Nb interfaces [8, 27, 37], all vacancy formation energies are positive, meaning that no constitutional vacancies are present in the ground state configuration of this Cu-Nb interface. Furthermore, all vacancies—even ones with lowest formation energies—retain the form of compact point defects and do not delocalize upon relaxation. In both the Cu and Nb interface atomic planes, areas of lowest vacancy formation energy are clustered into isolated patches. Comparing their location to the misfit dislocation network structure described in section III, we conclude that these patches coincide with intersections of set 3 misfit dislocations with set 1 and set 2 dislocations. Vacancy formation energies at intersections of set 3 dislocations with set 2 dislocations are about 0.2eV lower than at intersections between set 3 and set 1 dislocations.

Investigation of the formation energies of Cu, Nb, and He interstitials as well as He substitutionals yielded qualitatively similar insights to those gained from investigating vacancies: all formation energies are positive, no defect delocalization

takes place, and formation energies are lowest at intersections of set 3 misfit dislocations with set 1 and set 2 dislocations. Table II summarizes the point defect formation energies found at the Cu-Nb interface studied here.

VI. Discussion

The structure, shear resistance, and interaction with point defects determined for the interface studied here (termed Cu-Nb_{SPD}, for reference) may be compared to those of a different Cu-Nb interface found in magnetron sputtered multilayered composites (termed Cu-Nb_{MSP}). Experimental characterization has shown that the latter also forms in the Kurdjumov-Sachs orientation relation, defined by Eqn. 1 [15]. Crystallographically, Cu-Nb_{SPD} and Cu-Nb_{MSP} only differ in the orientation of their habit planes: $\{112\}_{fcc}||\{112\}_{bcc}$ for Cu-Nb_{SPD} and $\{111\}_{fcc}||\{110\}_{bcc}$ for Cu-Nb_{MSP}. Cu-Nb_{MSP} has been exhaustively studied through atomistic modeling, including its structure [8, 27, 53], shear resistance [27-29], interaction with point defects [8, 27, 37, 41], as well as other properties, such as interaction with climbing dislocations [54]. Selected findings from these studies will be described below as needed. Further details may be found in the foregoing references.

As discussed in section III, Cu-Nb_{SPD} contains three sets of parallel misfit dislocations, though for a tilt approaching ~6.7° the spacing between dislocations in one of the three sets goes to infinity. The spacing between dislocations in the two other sets is about 1-2nm and comparatively insensitive to tilt. Cu-Nb_{MSP} contains two sets of misfit dislocations whose spacing is also in the range of 1-2nm [8, 27]. Neither Cu-Nb_{SPD} nor Cu-Nb_{MSP} is coherent or even contains patches of coherency larger than about $2nm^2$. Furthermore, the misfit dislocations in both are so close to each other that they nearly overlap. Indeed, components of some of these dislocations are at least partially overlapping, as in the case of set 3 in Cu-Nb_{SPD} or set 2 in Cu-Nb_{MSP} [27]. Cu-Nb_{SPD} and Cu-Nb_{MSP} are therefore on the border between being describable as semicoherent and simply incoherent.

Despite these qualitative similarities in structure, the shear resistance of these interfaces and their interactions with point defects are markedly different. As shown in section IV, Cu-Nb_{SPD} shears in one direction (the x-direction) at an applied stress of ~1200MPa or less and not at all in the other (z) direction. The shear resistance of Cu-Nb_{MSP} is also anisotropic, but this interface does shear in all directions at applied stresses not exceeding ~1200MPa [27, 29]. Modeling predictions for Cu-Nb_{MSP} were experimentally confirmed in compression tests on pillars micromachined from Cu-Nb multilayers [55]. The Cu and Nb layers in these tests were oriented at an angle to the loading axis to maximize the resolved shear stress acting on the interface during compression.

The differing shear responses of these two interfaces may at first be thought to arise from discrepancies in interface energy: the ground state energy of Cu-Nb_{MSP} is ~540mJ/m^2 [8, 27] while that of Cu-Nb_{SPD} ranges from 690 to 820mJ/m^2, depending

on tilt angle (see section III). The effect of atomic bonding on shear resistance in Cu-Nb_{MSP} was investigated previously, however, using interatomic potentials tuned to give dilute heats of mixing of Cu in Nb and Nb in Cu ranging from highly negative (-0.5eV/atom) to highly positive (1.5eV/atom, well in excess of the dilute heats of mixing in the real Cu-Nb binary system [56]). It was found that the strength of bonding between Cu and Nb alters the numerical value of shear resistance of Cu-Nb_{MSP}, but does not change the mechanisms of interface shearing. In particular, Cu-Nb_{MSP} is able shear in all directions for all heats of mixing investigated [57].

These results suggest that the unlike shear responses of Cu-Nb_{SPD} and Cu-Nb_{MSP} do not arise from differences in bonding across the differing planes of these two interfaces. Their shear responses may, however, be understood on the basis of quantitative differences in their detailed misfit dislocation structure. Both sets of misfit dislocations in Cu-Nb_{MSP} have Burgers vectors that lie entirely within the interface plane [8, 27]. Since Burgers vectors of set 1 misfit dislocations are not parallel to those of set 2 in Cu-Nb_{MSP}, glide of these two sets of dislocations may lead to shearing of this interface in any direction.

By contrast, only one set of misfit dislocations in Cu-Nb_{SPD} has a Burgers vector that lies entirely within the interface plane, namely set 3. Furthermore, this Burgers vector is aligned with the x-direction. Glide of set 3 misfit dislocations within Cu-Nb_{SPD} is therefore able to account for shearing of Cu-Nb_{SPD} along the x-direction. This view is consistent with the disregistry plotted in Fig. 8, which shows lines of localized shearing in the x-direction whose orientation and spacing agrees with the predicted orientation and spacing of set 3 misfit dislocations in Cu-Nb_{SPD}.

The Burgers vectors of set 1 and 2 misfit dislocations in Cu-Nb_{SPD} both have components normal to the interface plane, i.e. the y-direction (see Table I). Thus, these misfit dislocations may not move within the interface plane by glide alone: climb within the interface would also have to occur and that would require mass transport into or out of these dislocations. Recent studies on the thermal stability of Cu-Nb ADB nanocomposites shed light on the likelihood of climb of interface misfit dislocations under high temperature. These studies were performed by in-situ heat-treatment under high energy synchrotron x-rays at the European Synchrotron Radiation Facility (ESRF, Grenoble, France) [58]. At 800°C, i.e. 0.8 of the thermodynamic melting temperature and 400-500°C above the classical recrystallization temperature, nanoscale Cu channels that are in contact with Nb nanofilaments via Cu-Nb_{SPD} interfaces do not fully relax their internal strain nor do they exhibit recrystallization by grain growth or thermal twinning.

Thus, conditions under which Cu-Nb_{SPD} interfaces may slide in the y-direction seem to be experimentally very difficult to meet. Indeed, the presence of highly stable Cu-Nb_{SPD} interfaces has been invoked to explain the observed unexpected thermal stability of the Cu nanochannels [58] and the present study appears to support this view. The effect of the emission of arrays of defects upon shearing in the y-direction (see Fig. 7) on microstructure development in these composites is unclear.

Both Cu-Nb_{SPD} and Cu-Nb_{MSP} are excellent trapping sites for vacancies, interstitials, and He impurities, as evidenced by the high binding energies of these defects at the interfaces [8, 27, 41]. Moreover, in both interfaces, the most favorable sites for defect trapping are the intersections between misfit dislocations. Both interfaces exhibit enhanced vacancy-interstitial recombination upon preloading with interstitials, similar to what has been observed in Cu grain boundaries [59].

Nevertheless, there are several differences between point defect behaviors at these two interfaces. First, when absorbed at misfit dislocations in Cu-Nb_{MSP}, vacancies and interstitials delocalize into extended defect configurations. No such delocalization occurs in Cu-Nb_{SPD}: vacancies and interstitials absorbed at misfit dislocations in this interface remain compact, just like conventional point defects in crystalline solids. Second, similar to certain grain boundaries in semiconductors [45, 46] and ceramics [60], Cu-Nb_{MSP} contains constitutional vacancies. Such vacancies are thermodynamically stable even at zero temperature because they are an intrinsic feature of the ground state interface configuration. In Cu-Nb_{MSP}, the concentration of constitutional vacancies is about atomic 5%. It gives rise to high excess volume, which is thought to enable these interfaces to absorb large quantities of implanted He without forming visible bubbles [37]. On the other hand, as shown in section V, Cu-Nb_{SPD} does not contain any constitutional defects.

Detailed analyses have revealed that delocalization of vacancies and interstitials at Cu-Nb_{MSP} is due to the reconstruction of these defects into combinations of kinks and jogs on pre-existing misfit dislocations [8, 27]. This delocalization mechanism, however, relies on the fact that one set of misfit dislocations in Cu-Nb_{MSP} is of nearly perfect screw character. All three sets of misfit dislocations in Cu-Nb_{SPD} have a significant edge component (see Table I), however, so the defect delocalization mechanism seen in Cu-Nb_{MSP} may not operate. The structure of delocalized vacancies and interstitials in Cu-Nb_{MSP} furthermore gives rise to a defect migration mechanism that restricts diffusion to one dimension [61]. Because vacancies and interstitials absorbed at Cu-Nb_{SPD} do not delocalize, they may be expected to migrate in all directions within the interface by conventional mechanisms.

The presence of constitutional vacancies at Cu-Nb_{MSP} may also be explained by reference to misfit dislocation structure. It has been shown that Cu-Nb_{MSP} can take on at least two distinct defect-free configurations that only differ by the location of one set of interface misfit dislocations [8, 27, 53]. In one of the two configurations, both sets of misfit dislocations reside in the Cu-Nb_{MSP} interface plane. In the other, one set of misfit dislocations resides in the Cu layer, one atomic plane spacing away from the interface plane. Although the difference in location of this set of misfit dislocations gives rise to a coherency strain in one atomic plane, the two interface configurations have nearly identical interface energies because energetically costly intersections between misfit dislocations are avoided in the latter configuration.

An interface configuration of lower energy than either of the defect free ones, however, arises when one set of misfit dislocations meanders between the interface plane and the neighboring Cu layer so as to both avoid intersecting other misfit dislocations *and* minimize coherency strains [8, 27]. The locations where the position of these dislocations changes from the interface plane to the Cu layer contain kink/jog configurations such as those found in Cu-Nb_{MSP} upon trapping and delocalization of vacancies. They therefore require the removal of an atom to form, explaining the presence of constitutional vacancies in Cu-Nb_{MSP}.

The lack of such vacancies in Cu-Nb_{SPD} may therefore be a consequence of the inability of misfit dislocations in this interface to exist outside the interface plane without incurring a significant energy penalty. This in turn may be because the habit planes of Cu-Nb_{SPD}, namely $\{112\}_{fcc}||\{112\}_{bcc}$, are not conventional glide planes in either of the adjoining crystals, unlike the habit planes in Cu-Nb_{MSP}: $\{111\}_{fcc}||\{110\}_{bcc}$. The absence of constitutional vacancies in Cu-Nb_{SPD} may influence its ability to delay the formation of bubbles under He implantation. This topic is currently under investigation by the authors.

The foregoing discussion shows that despite qualitative similarities between the structure of Cu-Nb_{MSP} and Cu-Nb_{SPD}, there are major differences in the shear response of these interfaces as well as in their interaction with point defects. These differences, however, may be explained based on quantitative details of misfit dislocation structure in these two interfaces. Thus, with a sufficient understanding of the mechanisms governing mechanical response and transport at interfaces, it may be possible to predict the properties of heterophase interfaces based on their misfit dislocation structure. Certain features of this structure may, in turn, be computed analytically from interface crystallography using well-known approaches such as the Frank-Bilby formalism used in section III [1, 27]. Continued improvements in the scope and precision of analytical interface structure models, such as the incorporation of interface disconnections, kinks, and jogs [62], may extend the range of interface properties that can be predicted. The appropriate choice of reference state in calculations involving the Frank-Bilby equation has also recently received attention [63].

Finally, there are numerous types of interfaces in ADB Cu-Nb nanocomposites other than the one investigated here. The bcc Nb nanofilaments in these materials are facetted [21], so Cu-Nb interfaces with the Kurdjumov-Sachs orientation relation (Eqn. 1), but interface planes other than $\{112\}_{fcc}||\{112\}_{bcc}$, may be found. Furthermore, besides the predominant $<111>_{Cu}$ texture component parallel to the wire axis, the Cu grains exhibit a second, minor texture component, namely $<100>_{Cu}$. The orientation relation of a fraction of the Cu-Nb interfaces in ADB composites may therefore be expected to differ from Kurdjumov-Sachs. HRTEM studies are currently being performed to characterize these different types of interfaces. From the present results, it may be anticipated that different atomic configurations will be characterized by different misfit dislocation structures and therefore possibly

different responses to shear and interactions with point defects. Further study of ADB Cu-Nb nanocomposites is expected to shed light on these differences.

VII. Conclusions

We presented an atomistic modeling study of the structure, shear response, and interaction with point defects of a Cu-Nb interface that has been observed in composites synthesized by wire drawing and accumulated roll bonding. This interface forms along $\{112\}_{Cu}||\{112\}_{Nb}$ atomic planes in the Kurdjumov-Sachs orientation relation (Eqn. 1). Our main conclusions are:

- The structure of this interface may be described using the misfit dislocation model: it contains three sets of closely spaced parallel misfit dislocations.
- This interface shears in one direction at applied stresses of below 1200MPa, but does not shear at all in the other direction. Instead, loading in the other direction leads to the emission of Shockley partial dislocations from the interface or extension or pre-existing ones.
- Vacancies, interstitials, and He impurities are trapped at misfit dislocation intersections in this interface. There is, however, no point defect delocalization nor does the interface contain any constitutional defects.
- The shear resistance and point defect interactions of this interface differ markedly from those of another kind of Cu-Nb interface found in magnetron sputtered multilayer composites, despite the fact that both interfaces are in the Kurdjumov-Sachs orientation relation and both contain closely spaced misfit dislocations.
- The different properties of these two interfaces may be explained in terms of quantitative differences in their detailed misfit dislocation structure, which arise because the two interfaces have different habit plane orientations.

VIII. Acknowledgements

This research was supported by the MISTI-France Seed Grant program at MIT. MJD thanks A. D. Rollett, J. Wang, I. J. Beyerlein, and N. Mara for insightful discussions. MJD and LT are grateful to D. Rodney for fruitful discussions. Investigations of point defect properties were supported by the Center for Materials in 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 award number 2008LANL1026. LT acknowledges the support of the French National Research Agency (ANR) under Contract ANR-06-MAPR-0013 and the French CNRS (accueil en délégation).

Figure Captions

Fig. 1: High resolution transmission electron microscopy (HRTEM) micrographs showing one Cu-Nb interface parallel to the wire axis. a) $\{111\}_{Cu}$ and $\{110\}_{Nb}$ planes are nearly parallel in adjacent Cu and Nb crystals. b) After image filtering, regularly spaced misfit compensating interfacial dislocations (black lines) are observed on the Cu side.

Fig. 2: Illustration of how atomic interface models were constructed.

Fig. 3: Visualization of the interface a) edge-on and b) in plan view. The dashed ellipses identify representative members of set 1 and 2 misfit dislocations in a) while the dashed lines in b) identify the possible line directions of set 3 dislocations (the thickest is considered the most likely direction, see text). Gray atoms are Nb, yellow are fcc Cu, blue are stacking faults in Cu, and red Shockley partial cores in Cu.

Fig. 4: Interface disregistry components plotted as a function of z.

Fig. 5: Visualization of the interface with a ~6.7° tilt imposed on the Cu side a) edge-on and b) in plan view. The dashed circle in a) identifies a representative set 1 misfit dislocation while the dashed line in b) is the most likely set 3 misfit dislocation direction. Note the absence of set 2 misfit dislocations (compare with Fig. 3). Gray atoms are Nb and yellow are Cu.

Fig. 6: Plots of stresses (top) and average displacement discontinuity across the interface $\Delta\vec{u}$ (bottom) for shearing of the interface shown in Fig. 3 along a) $-\hat{l} = -\frac{\sqrt{3}}{2}\hat{x} - \frac{1}{2}\hat{z}$ and b) $\hat{l} = \frac{\sqrt{3}}{2}\hat{x} + \frac{1}{2}\hat{z}$.

Fig. 7: a) The yield surface for shearing of the Cu-Nb interfaces studied here consists of two vertical lines at the critical σ_{xy} values at which slip in the x-direction initiates (lower for the interface without SPs shown in Fig. 5 than that with SPs in Fig. 3). b) Extension of SPs when $\sigma_{yz}\approx$-300MPa [see Fig. 6.a)]. c) Emission of defects when $\sigma_{yz}\approx$3800MPa. No slip occurs along the interface z-direction under any loading conditions. Gray atoms are Nb, yellow are fcc Cu, blue are Cu with local hcp symmetry, and red are SP cores in Cu. Two adjacent hcp planes in Cu denote an intrinsic stacking fault. Four adjacent hcp planes may result from the emission of two SPs separated by two atomic spacings.

Fig. 8: Slip across a CuNb interface with SPs is nonuniform, as evidenced by disregistry analysis. a) Slip begins at regions of low shear resistance, b), c) extends to adjacent areas, and c) links up into a system-wide slip pattern. The dashed line in d) indicates the predicted most likely direction of set 3 misfit dislocations in this interface (compare to Fig. 3).

Fig. 9: Vacancy formation energies as a function of distance from the Cu-Nb interface shown in Fig. 3. See text for descriptions of features marked with capital letters.

Fig. 10: Vacancy formation energy maps for interface atomic planes of a) Cu and b) Nb. The lowest formation energy sites are located at intersections of set 3 misfit dislocations with those of sets 1 and 2 [see Fig. 3.a)].

References

[1] Sutton AP, Balluffi RW. Interfaces in Crystalline Materials. Oxford: Oxford University Press, 1995.

[2] Misra A, Thilly L. Structural metals at extremes. MRS Bull. 2010;35:965.

[3] Rupert TJ, Trenkle JC, Schuh CA. Enhanced solid solution effects on the strength of nanocrystalline alloys. Acta Mater. 2011;59:1619.

[4] Rupert TJ, Schuh CA. Sliding wear of nanocrystalline Ni-W: Structural evolution and the apparent breakdown of Archard scaling. Acta Mater. 2010;58:4137.

[5] Schuh CA, Nieh TG, Iwasaki H. The effect of solid solution W additions on the mechanical properties of nanocrystalline Ni. Acta Mater. 2003;51:431.

[6] Hochbauer T, Misra A, Hattar K, Hoagland RG. Influence of interfaces on the storage of ion-implanted He in multilayered metallic composites. Journal of Applied Physics 2005;98:123516.

[7] Demkowicz MJ, Bellon P, Wirth BD. Atomic-scale design of radiation-tolerant nanocomposites. MRS Bull. 2010;35:992.

[8] Demkowicz MJ, Hoagland RG, Hirth JP. Interface Structure and Radiation Damage Resistance in Cu-Nb Multilayer Nanocomposites. Phys. Rev. Lett. 2008;100:136102.

[9] Misra A, Demkowicz MJ, Zhang X, Hoagland RG. The radiation damage tolerance of ultra-high strength nanolayered composites. Jom 2007;59:62.

[10] Medlin DL, Demkowicz MJ, Marquis EA. Solid State Interfaces: Toward an Atomistic-scale Understanding of Structure, Properties, and Behavior. Jom 2010;62:52.

[11] Dupouy F, Snoeck E, Casanove MJ, Roucau C, Peyrade JP, Askenazy S. Microstructural characterization of high strength and high conductivity nanocomposite wires. Scr. Mater. 1996;34:1067.

[12] Thilly L, Veron M, Ludwig O, Lecouturier F, Peyrade JP, Askenazy S. High-strength materials: in-situ investigations of dislocation behaviour in Cu-Nb multifilamentary nanostructured composites. Philos. Mag. A-Phys. Condens. Matter Struct. Defect Mech. Prop. 2002;82:925.

[13] Lim SCV, Rollett AD. Length scale effects on recrystallization and texture evolution in Cu layers of a roll-bonded Cu-Nb composite. Mater. Sci. Eng. A-Struct. Mater. Prop. Microstruct. Process. 2009;520:189.

[14] Lee S-B, LeDonne JE, Lim SCV, Beyerlein IJ, Rollett AD. The five-parameter heterophase interface character distributions (HICD) of physical vapor-deposited and accumulative roll-bonded Cu-Nb multilayer composites. Materials Science and Engineering A 2011;submitted.

[15] Mitchell TE, Lu YC, Griffin AJ, Nastasi M, Kung H. Structure and mechanical properties of copper/niobium multilayers. J. Am. Ceram. Soc. 1997;80:1673.

[16] Wang YC, Misra A, Hoagland RG. Fatigue properties of nanoscale Cu/Nb multilayers. Scr. Mater. 2006;54:1593.
[17] Misra A, Hoagland RG, Kung H. Thermal stability of self-supported nanolayered Cu/Nb films. Philos. Mag. 2004;84:1021.
[18] Misra A, Hirth JP, Hoagland RG, Embury JD, Kung H. Dislocation mechanisms and symmetric slip in rolled nano-scale metallic multilayers. Acta Mater. 2004;52:2387.
[19] Mara NA, Sergueeva A, Tamayo T, Zhang X, Misra A, Mukherjee A. High temperature mechanical properties of Cu/Nb nanoscale multilayers at diminishing length scales. Jom 2004;56:141.
[20] Spencer K, Lecouturier F, Thilly L, Embury JD. Established and emerging materials for use as high-field magnet conductors. Adv. Eng. Mater. 2004;6:290.
[21] Vidal V, Thilly L, Lecouturier F, Renault PO. Effects of size and geometry on the plasticity of high-strength copper/tantalum nanofilamentary conductors obtained by severe plastic deformation. Acta Mater. 2006;54:1063.
[22] Wood JT, Griffin AJ, Embury JD, Zhou R, Nastasi M, Veron M. The influence of microstructural scale on the combination of strength and electrical resistivity in copper based composites. J. Mech. Phys. Solids 1996;44:737.
[23] Lee KH, Hong SI. Interfacial structure of nanostructured Cu-Nb filamentary composite fabricated by the bundling and drawing process. Philos. Mag. Lett. 2004;84:515.
[24] Leprince-Wang Y, Han K, Huang Y, Yu-Zhang K. Microstructure in Cu-Nb microcomposites. Mater. Sci. Eng. A-Struct. Mater. Prop. Microstruct. Process. 2003;351:214.
[25] Hoagland RG, Hirth JP, Misra A. On the role of weak interfaces in blocking slip in nanoscale layered composites. Philos. Mag. 2006;86:3537.
[26] Hoagland RG, Kurtz RJ, Henager CH. Slip resistance of interfaces and the strength of metallic multilayer composites. Scr. Mater. 2004;50:775.
[27] Demkowicz MJ, Wang J, Hoagland RG. Interfaces between dissimilar crystalline solids. In: Hirth JP, editor. Dislocations in Solids, vol. 14. Amsterdam: Elsevier, 2008. p.141.
[28] Wang J, Hoagland RG, Hirth JP, Misra A. Atomistic modeling of the interaction of glide dislocations with "weak" interfaces. Acta Mater. 2008;56:5685.
[29] Wang J, Hoagland RG, Hirth JP, Misra A. Atomistic simulations of the shear strength and sliding mechanisms of copper-niobium interfaces. Acta Mater. 2008;56:3109.
[30] Mara NA, Bhattacharyya D, Dickerson P, Hoagland RG, Misra A. Deformability of ultrahigh strength 5 nm Cu/Nb nanolayered composites. Applied Physics Letters 2008;92:3.
[31] Mara NA, Bhattacharyya D, Hoagland RG, Misra A. Tensile behavior of 40 nm Cu/Nb nanoscale multilayers. Scr. Mater. 2008;58:874.
[32] Misra A, Hirth JP, Hoagland RG. Length-scale-dependent deformation mechanisms in incoherent metallic multilayered composites. Acta Mater. 2005;53:4817.

[33] Misra A, Hirth JP, Kung H. Single-dislocation-based strengthening mechanisms in nanoscale metallic multilayers. Philosophical Magazine A (Physics of Condensed Matter: Structure, Defects and Mechanical Properties) 2002;82:2935.
[34] Thilly L, Lecouturier F, von Stebut J. Size-induced enhanced mechanical properties of nanocomposite copper/niobium wires: nanoindentation study. Acta Mater. 2002;50:5049.
[35] Singh BN. Effect of grain size on void formation during high-energy electron irradiation of austenitic stainless steel. Philos. Mag. 1974;29:25.
[36] Zhang X, Fu EG, Misra A, Demkowicz MJ. Interface-enabled Defect Reduction in He Ion Irradiated Metallic Multilayers. Jom 2010;62:75.
[37] Demkowicz MJ, Bhattacharyya D, Usov I, Wang YQ, Nastasi M, Misra A. The effect of excess atomic volume on He bubble formation at fcc-bcc interfaces. Applied Physics Letters 2010;97.
[38] Zhernenkov M, Jablin MS, Misra A, Nastasi M, Wang Y-Q, Demkowicz MJ, Baldwin JK, Majewski J. Trapping of implanted He at Cu/Nb interfaces measured by neutron reflectometry. Applied Physics Letters 2011;98:241913.
[39] Kaufman L. Coupled phase diagrams and thermochemical data for transition metal binary systems-III. CALPHAD 1978;2:117.
[40] Daw MS, Baskes MI. Embedded-Atom Method - Derivation And Application To Impurities, Surfaces, And Other Defects In Metals. Phys. Rev. B 1984;29:6443.
[41] Demkowicz MJ, Hoagland RG. Simulations of collision cascades in Cu-Nb layered composites using an EAM interatomic potential. International Journal of Applied Mechanics 2009;1:421.
[42] Plimpton S. FAST PARALLEL ALGORITHMS FOR SHORT-RANGE MOLECULAR-DYNAMICS. J. Comput. Phys. 1995;117:1.
[43] Kurdjumov GV, Sachs G. Zeitschrift fur Physik 1930;64:325.
[44] Duesbery MS, Vitek V. Plastic anisotropy in bcc transition metals. Acta Mater. 1998;46:1481.
[45] von Alfthan S, Haynes PD, Kaski K, Sutton AP. Are the structures of twist grain boundaries in silicon ordered at 0 K? Phys. Rev. Lett. 2006;96:055505.
[46] von Alfthan S, Kaski K, Sutton AP. Order and structural units in simulations of twist grain boundaries in silicon at absolute zero. Physical Review B (Condensed Matter and Materials Physics) 2006;74:134101.
[47] Holm EA, Foiles SM. How Grain Growth Stops: A Mechanism for Grain-Growth Stagnation in Pure Materials. Science 2010;328:1138.
[48] Olmsted DL, Holm EA, Foiles SM. Survey of computed grain boundary properties in face-centered cubic metals-II: Grain boundary mobility. Acta Mater. 2009;57:3704.
[49] Hoagland RG, Mitchell TE, Hirth JP, Kung H. On the strengthening effects of interfaces in multilayer fcc metallic composites. Philos. Mag. A-Phys. Condens. Matter Struct. Defect Mech. Prop. 2002;82:643.
[50] Hirth JP, Lothe J. Theory of Dislocations. New York: Wiley, 1982.
[51] Knowles KM. The dislocation geometry of interphase boundaries. Philos. Mag. A-Phys. Condens. Matter Struct. Defect Mech. Prop. 1982;46:951.
[52] Kashinath A, Demkowicz MJ. A predictive interatomic potential for He in Cu and Nb. Model. Simul. Mater. Sci. Eng. 2011;19.

[53] Demkowicz MJ, Hoagland RG. Structure of Kurdjumov-Sachs interfaces in simulations of a copper-niobium bilayer. J. Nucl. Mater. 2008;372:45.
[54] Wang J, Hoagland RG, Misra A. Room-temperature dislocation climb in metallic interfaces. Applied Physics Letters 2009;94:131910.
[55] Mara NA, Bhattacharyya D, Hirth JP, Dickerson P, Misra A. Mechanism for shear banding in nanolayered composites. Applied Physics Letters 2010;97:021909.
[56] Liu XY, Hoagland RG, Wang J, Germann TC, Misra A. The influence of dilute heats of mixing on the atomic structures, defect energetics and mechanical properties of fcc-bcc interfaces. Acta Mater. 2010;58:4549.
[57] Wang J, Hoagland RG, Liu XY, Misra A. The influence of interface shear strength on the glide dislocation-interface interactions. Acta Mater. 2011;59:3164.
[58] Dubois JB, Thilly L, Renault PO, Lecouturier F, Di Michiel M. Thermal stability of nanocomposite metals: In situ observation of anomalous residual stress relaxation during annealing under synchrotron radiation. Acta Mater. 2010;58:6504.
[59] Bai XM, Voter AF, Hoagland RG, Nastasi M, Uberuaga BP. Efficient Annealing of Radiation Damage Near Grain Boundaries via Interstitial Emission. Science 2010;327:1631.
[60] Zhang ZL, Sigle W, Phillipp F, Ruhle M. Direct atom-resolved imaging of oxides and their grain boundaries. Science 2003;302:846.
[61] Kolluri K, Demkowicz MJ. Dislocation mechanism of interface point defect migration. Phys. Rev. B 2010;82.
[62] Hirth JP, Pond RC, Lothe J. Spacing defects and disconnections in grain boundaries. Acta Mater. 2007;55:5428.
[63] Hirth JP, Pond RC, Hoagland RG, Wang J, Demkowicz MJ, Liu XY. Interface Defects, Reference Spaces and the Frank-Bilby Equation. 2011;to be submitted.