Layer size effect on the shock compression behavior of fcc-bcc nanolaminates

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Abstract

Using large scale nonequilibrium molecular dynamics simulations, we study the role of interfaces and layer thickness in the response of the experimentally observed Cu/Nb nanolayered composites to shock compression. We observe a critical layer thickness (< 20 nm) below which lattice dislocations nucleate preferentially from the Cu/Nb interfaces. Within this regime of interface dominance, samples with a layer thickness of 5 nm have the largest Hugoniot elastic limit (the critical shock pressure required for dislocation production), which then decreases for finer layer thicknesses, where dislocation transmission across the interfaces becomes more frequent. The dislocation slip systems emitted and transmitted across the interfaces are strongly linked to interface structure and crystallography. The strong layer thickness and interface structure effects found here can provide insight into designing shock-resistant nanolayered composites.

Keywords: MD simulation, nanocomposites, interface, dislocation, shock compression

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I. Introduction

Materials for next generation applications are expected to push the envelope and exhibit predictable lifetime performance in extreme environments for longer service-lives than are attainable with today's materials. To this end, nanolayered composite metals have become an attractive candidate. Many experimental studies have shown that nanolayered metals exhibit extraordinary resiliency in extreme environments, such as high temperatures, radiation, stresses, and large strains, above and beyond that possible with their constituents alone [1] [2] [3] [4] [5]. These nanomaterials combine two or more dissimilar metals and contain an unusually high density of bimetal interfaces [5] [6] [7]. Recently, small-scale studies have been focused on the atomic structures of these bimetal interfaces and how they influence basic deformation processes, like dislocation nucleation and deformation twinning [8] [9]. From both experiment and simulation, it was found that these mechanisms were very sensitive to the structure of the interfaces at an atomic scale [5] [10] [11].

In order to determine how interface structure would contribute to composite response in an extreme environment, large scale nonequilibrium molecular dynamics (MD) simulations were carried out to investigate the effect of interface structure on shock compression response [12]. A three-dimensional model of single crystal multilayers was constructed with either a $\{112\}\text{fcc}||\{112\}\text{bcc}$ interface or a $\{111\}\text{fcc}||\{110\}\text{bcc}$ interface, both adopting a Kurdjumov-Sachs (KS) orientation relation. It was found that the pressure to initiate plasticity was twice as high in the $\{111\}\text{fcc}||\{110\}\text{bcc}$ KS nanocomposite than the $\{112\}\text{fcc}||\{112\}\text{bcc}$ KS nanocomposite [12]. The difference was attributed to differences in the stresses required to nucleate and transmit dislocations across the interface. This result implies that atomic structure plays a key role in interface-driven plasticity.

A question that remains concerns layer size effects on high-rate deformation plasticity. It has been demonstrated in several experimental studies that layer size significantly impacts the hardness and strength of multilayers [13] [1]. It has been shown in a recent experimental

study that nanocrystal size greatly affects the propensity for nanomaterials to deformation twin [14]. Based on dislocation theory, it has been proposed that layer thickness has a profound effect on the plastic deformation mechanism, from confined layer slip to interface crossing [13]. Both experimental and simulation studies have observed a cross-over from full dislocation-mediated to partial-dislocation mediated slip as the crystal size reduces below a critical value [15] [16] [17] [18]. In FCC metals, the effect of grain size on dislocations generated from grain boundaries were analyzed using MD simulation by Asaro et al. [19] and Traiviratana et al. [20]. Using phase-field dislocation dynamics, nanograin sizes have also been found to influence the size of the stacking faults that are emitted from grain boundaries [21]. Many of these size effects arise because of changes in where dislocations nucleate and whether they can transmit across the interfaces.

In this work, we apply large scale nonequilibrium MD simulations to Cu-Nb nanolayers as a prototype for examining the effect of layer size on the interface-mediated processes during shock compression. To this end, we first construct a new Cu-Nb interatomic potential for Cu and Nb potentials proven to provide accurate defect dynamics under high pressure. We show that there are two important length scales affecting shock compression behavior, one below which interface-mediated dislocation nucleation dominates, and another below which dislocation transmission becomes more frequent. The latter gives rise to a peak Hugoniot elastic limit (critical shock pressure) for a 5 nm layer thickness.

II. Strategy and Methodology

A. Construction of Cu-Nb cross potential

Some interatomic potentials for bcc metals, such as Nb, can exhibit artificial structural phase transformations under high pressure, making them unsuitable for shock compression studies [22] [23]. In prior work, we have shown that the origin can be traced to artificial minima in the material gamma surfaces under extreme pressures [23]. After comparing different potentials developed for Nb, we found that the one developed by Ackland and

Thetford best describes the high-pressure response, providing a good description of Nb deformation twinning and other defect-related properties. Therefore, here we adopt the embedded atom method (EAM) potential developed by Voter and Chen [24] for fcc Cu, and the Finnis-Sinclair (FS) potential by Ackland and Thetford [25] for bcc Nb. Development of the cross potential between Cu and Nb is accomplished by the following procedure.

We employ the same fitting scheme as proposed by Demkowicz et al. [26] but use Ackland FS Nb potential in place of the Johnson EAM Nb potential [26]. The interaction between Cu and Nb is described by a two-body Morse potential,

$$\bar{f}_{CuNb}(r) = D_M (1 - e^{\bar{a}_M (r - R_M)})^2 - D_M, \quad (1)$$

where r is the interatomic distance, and D_M , a_M and R_M are three fitting constants. In addition, two transformation invariants were taken into consideration,

$$F^{new}(\bar{r}) = F(\bar{r}) + g\bar{r}, \quad f^{new}(r) = \bar{f}(r) - 2gr(r), \quad (2)$$

and

$$r^{new}(r) = sr(r), \quad F^{new}(\bar{r}) = F(\bar{r}/s), \quad (3)$$

which adds three more fitting constants, g_{Cu} , g_{Nb} , and s_{Nb} .

Due to the immiscibility of Cu/Nb, there are no equilibrium compounds that can be used for fitting the cross potential. To overcome this, first-principles calculations are first performed to obtain some fundamental properties of the B1(NaCl) and B2(CsCl) structures, e.g., lattice parameters, formation enthalpies and elastic constants. These were then used in the fitting procedure. Table I lists the fitted and reproduced properties of the newly constructed cross potential for the Cu/Nb system. The latter are found to compare well with both experimental values and *ab initio* density functional theory (DFT) values for the lattice parameters, cohesive energies and elastic constants of the pure metals and some selected compounds [27] [28] [29]. As will be shown in the next section, the new cross-potential

provides estimates of interfacial energy and structure in agreement with those of previous Cu/Nb potentials [26].

B. MD modeling and simulation

In the present study, we consider Cu/Nb interfaces, which have the crystallographic character commonly observed in physical vapor deposited foils [30] [31]. Our models are created by joining a {111} slab of perfect fcc Cu with a {110} slab of perfect bcc Nb in a KS orientation relationship, meaning the planes (111)Cu//(110)Nb are aligned, as are the [1-10]Cu//[-111]Nb and [11-2]Cu//[1-12]Nb axis pairs in the plane of the interface. The x-axis is along the [11-2]Cu direction, the y-axis is along the [1-10]Cu direction, and the z-axis is along the [111]Cu direction. The interface planes are then parallel to the x-y plane. The multilayer interface models terminate at the free surfaces at both sides of the model. Periodic boundary conditions are applied in the x and y directions, whose dimensions are chosen such that the absolute strains imposed on Cu and Nb semi-infinite perfect crystals are minimized [32] [33]. Four types of Cu/Nb multilayer models with different layer thickness (2.5 nm, 5 nm, 10 nm and 20 nm) are constructed to study the effect of layer thickness on the formation of defective structure. For each layer thickness, the total sample length in the shock direction is about 120 nm, giving total sample sizes ranging from about 3 to 4 million atoms. This initial multilayer model is first relaxed by a quenching MD method combined with a conjugate gradient algorithm. Afterwards, an Isothermal-Isobaric (NPT) ensemble is applied to equilibrate the sample at zero pressure and the desired 300 K target temperature. After these procedures, the relaxed multilayered models are used for the shock compression and release studies using the Scalable Parallel Short-range Molecular dynamics code (SPaSM) [34] [35] [36].

A shock wave is then introduced by impacting the sample at the specified piston (or particle) velocity u_p against a stationary specularly reflecting wall, i.e., the so-called momentum mirror method which has been used to study the homogenous nucleation of

dislocations [36] [37], twins [38], and phase transformations [39] in defect-free single crystals. No additional coupling of the atoms to a heat bath is done, since shock waves are assumed to be adiabatic i.e., occurring too fast for any heat exchange with the environment [40] [39]. The piston velocity u_p is varied to find a rough critical threshold at which the defective structure first appears in the samples, i.e. the Hugoniot elastic limit. Because there are no pre-existing (threading) defects within the layers, the critical pressure corresponds to that needed to nucleate fresh dislocations either within the layers or from the interfaces, under the uniaxial strain state created by the initial elastic shock compression.

For better on-the-fly visualization, the centro-symmetry factor (CSF) is used to identify defects during the course of shock propagation using the MD_RENDER code [41]. The CSF parameter is a quantitative measure of the deviation from the ideal centro-symmetry in the atom's neighborhood. It can be defined as [42] $P = \frac{1}{N_p} \sum_{i=1}^{N_p} \left| \mathbf{r}_i + \mathbf{r}_{i+N_p} \right|^2$, where $\mathbf{r}_i$ and $\mathbf{r}_{i+N_p}$ are positions of the i th pair of neighbors relative to the atom under consideration. In this summation, the number of nearest-neighbor pairs N_p depends on the host crystal structure: N_p is 6 for FCC and 4 for BCC. For perfect FCC (or BCC) structures, vectors $\mathbf{r}_i$ and $\mathbf{r}_{i+N_p}$ in each neighbor pair cancel each other so that P vanishes for every atom. To distinguish Shockley partial dislocations in an fcc crystal, we also use common neighbor analysis (CNA).

III. Results and Discussions

A. Interface structure

Fig. 1 (a)-(b) shows the relaxed atomic Cu/Nb interface structure that is obtained by relaxing a bi-crystal using the newly constructed Cu/Nb potentials. Besides the quantitative difference in interface formation energy, 669 mJ/m² using the newly constructed Cu/Nb potentials and 569 mJ/m² [43] using the cross-pair potential by Demkowicz et al. [26], we obtained the same interface structure as reported previously by our team [44] [32]. Cu and Nb form a sharp interface without intermixing. The atoms marked by magenta and red colors

indicate misfit dislocation intersections (MDIs). These MDIs coincide with the points where the two separate intrinsic dislocation arrays intersect [45]. As indicated by the parallelogram in Fig. 1b, the MDIs exhibit a quasi-repeatable pattern of a two-dimensional boundary unit cell (BUC). Using interface defect analyses, two sets of misfit dislocation arrays have been identified, as indicated by the dashed lines in Fig. 1a [33] [11] [46]. The line orientations and Burgers vectors for these misfits have been characterized in [33]. The first dislocation array has line sense $\xi_1 = (\cos 28^\circ, \sin 28^\circ)$, a spacing of 21.3 Å, and a Burgers vector of (0, 2.70) Å. The second array has line sense $\xi_2 = (\cos 90^\circ, \sin 90^\circ)$, a spacing of 12.45 Å, and a Burgers vector of (-2.45, 1.56) Å.

Recently, it was shown that this misfit dislocation network plays a key role in the nucleation of dislocations from the interface under quasistatic mechanical loading [9] [11] [47]. Dislocation loops are emitted along the crystallographic slip planes that intersect the interface plane along the misfit dislocation lines, but do not form on planes that do not satisfy this criterion despite being equally stressed. On this basis, for later reference, we illustrate some geometric relationships between this misfit dislocation network and the dislocation glide planes in Cu and Nb. Fig. 1c shows the unfolded tetrahedron of slip systems out of the interface on the Cu side, in which the three fcc glide planes are marked by BCD, ACD, ABD planes, and the plane ABC corresponds to the Cu/Nb interface plane. Likewise, the 2D representation of an unfolded polyhedron of the relevant slip systems out of the interface on the Nb side is shown in Fig. 1d, in which the five bcc glide planes are indicated by B'C'F', A'C'G, A'C'G', A'B'E, A'B'E' planes, and the plane A'B'C' corresponds to the Cu/Nb interface plane. The dislocation line ξ_1 is nearly parallel to the AC trace of glide plane ACD in the Cu side, but slightly deviates from the A'C' trace of glide planes A'C'G and A'C'G'. Meanwhile, the dislocation line ξ_2 is exactly parallel to the AB trace of glide plane ABD on the Cu side, and the **A'B' trace** of glide plane A'B'E (or A'B'E') on the Nb side. According to the theory in [9] [11], these planes are candidates for dislocation nucleation, whereas the

others are not. We will further observe here that these geometric orientation relationships between the adjoining crystals and their common interface also greatly impact dislocation nucleation as well as dislocation transmission across the interface during shock compression.

B. Dislocation nucleation at interface

Interfaces are expected to dominant plastic deformation as the interface spacing h decreases, or the interface density increases. Such critical length scales are often associated with reduced defect content and suppression of pile-ups within the layers or enhanced stress states that are generated as crystalline sizes shrink to very fine scales (e.g., < 10 nm). We first explore the effect of interface spacing h (or layer thickness) on where plasticity initiates in an otherwise pristine composite. Two critical length scales are observed.

The first is the length scale between $h = 10$ nm and 20 nm, where dislocation nucleation transitions from occurring within the layers to at the interfaces. As shown in Fig. 2 (a)-(c), it is observed that fcc Shockley partial dislocation loops are emitted from the Cu/Nb interface into Cu for the Cu 2.5/Nb 2.5nm, Cu 5nm/Nb 5nm and Cu 10nm/Nb 10nm models at critical piston speeds of $u_p = 625, 650$ and 625 m/s, respectively. Nucleation into Cu from the interface is preferred over Nb since Cu dislocations have the smaller Burgers vector and self-energy [48]. In contrast, for the thicker Cu 20nm/Nb20nm model and for comparison, a bulk Nb crystal, a dislocation loop first appears inside the Nb layer at $u_p = 615$ m/s and 600 m/s, respectively. Fig. 2(d) and (e) shows the initial stage of this homogeneous dislocation nucleation within one Nb layer.

To see how this size effect manifests later in deformation, Fig. 3 shows snapshots of the (a) 2.5 nm, (b) 5 nm, (c) 10 nm, and (d) 20 nm multilayers at the time of 19.5 ps, near the end of the shock compression stage. For all layer thicknesses, the sample is travelling at a particle velocity $u_p = 650$ m/s. Shockley partials are largely responsible for plastic deformation in the Cu layers for all thicknesses. In the Nb layers, twins and slip dislocations can be identified for

thicker layered composite 20 nm (see Fig. 3c and 3d), and only slip dislocations in all the remaining finer layers.

The second important size effect corresponds to the layer thicknesses of 5 nm, where the threshold for interface-driven plasticity achieves a peak value. This critical value for the onset of plastic yield involves the motion of the first set of dislocations formed, including their nucleation, propagation, and transmission of dislocations across interfaces. A similar size effect in strength is seen in hardness testing of these Cu-Nb multilayers via room-temperature and high-temperature nano-indentation, also applied normal to the interfaces [49] [13] [1] [50]. There, a peak hardness is achieved also at $h \sim 5$ nm and is presumed to correspond to the length scale at which interface crossing prevails.

For the case of the 5 nm composite, Fig. 4a shows a snapshot of dislocation nucleation from the interface into the Cu crystal at an incipient stage at 6.5 ps. To expose the relationship with the interface misfit dislocation network, Fig. 4b shows the top view of this nucleation event from the Cu side, where the dashed orange lines indicate a few misfit dislocation lines. For this particular loading state, three Shockley partial dislocations that can form an intrinsic stacking fault as it propagates away from the interface have the same Schmid factor. With the passage of shock compression wave, however, only one partial dislocation loop expands, as seen in Fig. 4c and 4d, while the other two appear to be hindered. The preferred partial dislocation loop nucleates along the misfit dislocation line ξ_1 , which is nearly aligned with the trace of glide plane of ACD at interface (Fig. 1a,c). As mentioned, the preference for dislocations to nucleate along misfit dislocation lines was reported previously in other MD simulations in uniform loading [48] and has been predicted by a geometric based model [11]. The prevalence of this nucleation mechanism among simulations carried out at different strain rates and temperatures highlights the strong relationship between the intrinsic misfit dislocation network and interface driven plasticity.

Last, we note that with continued shock propagation, the trailing Shockley partial dislocation is emitted from the interface (Fig. 4c). The leading and trailing partials form an extended full dislocation that is mobile in the Cu crystal.

C. Dislocation transmission at interface

After dislocations nucleate, they expand and reach the neighboring interfaces where they either are absorbed or transmit across the interfaces. The transmission of dislocations across this particular interface has been shown to be difficult [32]. Atomic-scale simulations have found that the core of the absorbed dislocation tends to spread in the plane of the interface, which greatly hinders its re-emission into the adjoining crystals, which would complete the transmission process. Another factor that influences transmissibility is the degree of alignment of the slip planes and Burgers vectors that make up the transmission pathway of the dislocation [51] [8]. Whether two slip systems across an interface are sufficiently well aligned for dislocation transmission has been measured by a geometry factor. This factor, designated as m' , can be calculated from two angles: the angle ϕ , between the slip directions b and b' and the angle λ , between the normals n and n' to the slip planes (see Fig. 5). The geometric compatibility factor m' , is calculated as $m' = (\cos \phi) (\cos \lambda)$, which varies from 0 to 1, with 1 being a perfectly aligned transmission path.

Fig. 6a shows the relative orientation of the FCC and BCC active slip systems with respect to the Cu/Nb KS interface. Fig. 6b gives the top view of the interface together with the traces of active glide planes on the interface: black ABC' is for the Nb side and pink ABC for Cu. Only one set of $\{111\}$ Cu and $\{110\}$ Nb glide planes share a common trace of AB ($\langle 1-10 \rangle$) at the interface. The compatibility factor m' for transmission to and from the ACD glide plane in Cu and the glide A'C'G' plane in Nb is calculated to be 0.66, which is much larger than the other possible transmission paths to A'C'G ($m' = 0.056$), B'C'F' ($m' = 0.035$ and 0.27), A'B'E ($m' = 0.392$), and A'B'E' ($m' = 0.021$).

Fig. 7a shows a dislocation transmission event from the Cu side of an interface into the Nb side. In this figure, the sample is travelling upwards at a particle velocity $u_p = 650$ m/s towards a stationary piston at the top, and the resulting shockwave travels downward. The Cu and Nb slip systems involved correspond to those with the highest m' : ACD (on the Cu side) and A'C'G' (on the Nb side) (refer to Fig. 1c and 1d for slip systems).

In a similar manner, the dislocation in Nb has propagated to the opposing interface and has transmitted into Cu. Again, the transmission pathway corresponds to the one with the highest compatibility factor m' , i.e., from an active glide plane of A'C'G' in the Nb layer onto the ACD glide plane in the Cu layer.

At the transmission site, a residual dislocation is left behind within the interface. Fig. 8 shows an example of the local disruption of the interface atomic structure after a single transmission event. As plastic deformation develops in the layers (Fig. 4), slip transmission appears to become less frequent. Transmission can become increasingly more difficult for many reasons: accumulated changes in interface structure (e.g., Fig. 8), backstresses by extrinsic dislocations stored in the interface [52], and changes in interface character and hence m' as either crystal reorients during deformation.

D. Dislocation absorption and annihilation at interface

Finally we examine the evolution of the shock-induced defects during the shock release to gain some clues on interface-mediated recovery. It may be expected that when the shock wave reaches the free surface and a rarefaction (relief) wave is produced, the stacking faults that were produced in shock compression could be mostly annihilated. This idea is consistent with the observation of much smaller dislocation densities in recovered shocked materials [53]. Although quantitative comparison of dislocation density between those predicted in MD simulations and experiments is still far beyond expectation, some qualitative trends may be considered intuitively useful. For instance, previously shock simulations of single crystals without initial defects have been carried out [54]. When comparing the calculated density of

defects with post-mortem observations on recovered single crystal Cu, it was found that the dislocation densities in the simulations were several orders of magnitude lower [53]. Three reasons were suggested by Cao et al. [53] for the **discrepancy**: (a) the higher strain rate and much shorter rise time in the MD simulations, (b) the small volume of the model single crystal, and (c) the possibility that most defects are annealed out in the simulations.

The present MD simulations on nanolayered samples are found not to follow exactly the same trend as those performed on the single crystals due to the presence of interfaces. To examine defect evolution, Fig. 9 shows the change in the atomic percentage of central symmetry factor (CSF) greater than unity (corresponding to defects) for the Cu 5nm/Nb 5nm multilayer model. It can be clearly seen that the peak defect density is reduced by ~30% during the initial shock release stage, with only a negligible further decrease during the subsequent annealing process. **We observe that most of the defect substructures inside Nb are recovered during the shock relief process, while the substructure inside the fcc-Cu layers is only partially recovered during shock release of the multilayered Cu-Nb nanocomposites. At the same time, we find that** the originally planar interfaces have been significantly altered by the numerous dislocation-interface interactions (primarily emission and transmission) during shock compression. This change in interface structure may be one reason why the shock-induced defects are not fully recovered. This result may shed light on why it has been reported that voids initiate in the Cu phase rather than the Nb phase during shock testing of these nanolayers [55].

IV. Conclusions

In this work, we used atomic scale MD simulations to study the response of Cu/Nb nanolayered composites to shock compression. Construction of a reliable MD model for this extreme pressure environment required development of a Cu-Nb cross potential derived using the Voter-Chen Cu and Ackland Nb potentials. The energy and atomic structure of the KS

Cu/Nb interfaces with the new cross-potential are shown to be in agreement with those reported previously. The main conclusions of this work are as follows:

- Under shock compression, we reveal a critical layer thickness (< 20 nm) below which lattice dislocations nucleate preferentially from the Cu/Nb KS interfaces.
- A peak in the Hugoniot elastic limit (resistance to shock-induced plasticity) is found for a layer thickness of 5 nm, below which dislocation transmission across the interface becomes more frequent.
- The preferred transmission pathways to and from Cu and Nb crystals abide by the simple geometric factor that measures the degree of alignment of slip systems across an interface.
- Most of the dislocation substructures formed within the layers during shock compression are recovered in Nb but not in Cu, which we suspect is a result of a change in the interface morphology and defect content during shock compression.

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TABLE I. The fitted properties of the newly constructed Cu/Nb cross potential. These are compared with values from experiment, previous Cu-Nb potentials, and ab initio DFT. The lattice parameter a is given in Å, the cohesive energy E_c in eV, dilute heats of mixing in eV, and the interfacial energy in mJ/m². **KS indicate Kurdjumov-Sachs fcc/bcc interfaces.**

	Elements		Compounds			
	Cu	Nb	B1	B2	L1 ₂ -Cu ₃ Nb	L1 ₂ -CuNb ₃
a	3.62	3.30	4.92	3.15	3.78	4.01
	3.62 [#]	3.30 [#]	5.19 [#]	3.19 [#]	3.84 [#]	4.10 [#]
	3.62 [*]	3.30 [*]	-	3.12 ^{\$}	3.81 ^{\$}	4.05 ^{\$}
E _c	3.54	7.57	5.33	5.55	4.47	6.34
	3.54 [#]	7.47 [#]	4.87 [#]	5.48 [#]	4.39 [#]	6.22 [#]
	3.48 [*]	7.57 [*]	-	5.35 ^{\$}	4.18 ^{\$}	6.40 ^{\$}
C ₁₁	179	247	286	194	154	90
	179 [#]	243 [#]	567 [#]	225 [#]	219 [#]	173 [#]
	168 [*]	247 [*]	-	166 ^{\$}	154 ^{\$}	94 ^{\$}
C ₁₂	123	133	117	132	129	140
	123 [#]	134 [#]	98 [#]	181 [#]	171 [#]	126 [#]
	122 [*]	135 [*]	-	170 ^{\$}	146 ^{\$}	192 ^{\$}
C ₄₄	81	28	32	47	59	60
	81 [#]	30 [#]	11 [#]	117 [#]	99 [#]	53 [#]
	76 [*]	29 [*]	-	48 ^{\$}	48 ^{\$}	44 ^{\$}
Dilute heats of mixing				Interfacial energies		
Nb in Cu	1.05		KS		668	
	1.02 ^{&} , 1.03 [#]				574 [#]	
Cu in Nb	0.56					
	0.48 ^{&} , 0.44 [#]					

* The experimental data are from Ref. [27]

\$ The ab initio DFT values from [28]

& Derived from phase diagram thermodynamic calculations [29]

The calculated values by the previous Cu-Nb potentials by Demkowicz et al. [26]

Figure Captions

FIG. 1 (color online). The atomic structure of the Cu/Nb interface with the KS orientation relationship after NPT and quenching relaxation (a) top view from the Cu side and (b) bottom view from the Nb side. The interfacial MDIs are indicated by magenta and red color. (c) Two-dimensional representation of the unfolded tetrahedron of slip systems out of the interface in the Cu side, in which the three gliding planes are indicated by the BCD, ACD, and ABD planes, and the ABC plane is the Cu/Nb interface. (d) Two-dimensional representation of an unfolded polyhedron of slip systems out of the interface in the Nb side, in which the five relevant gliding planes are indicated by B'C'F', A'C'G, ACG', A'B'E, A'B'E' planes, and the Cu/Nb interface is located at the A'B'C' plane. The interface normal is $[111]_{\text{Cu}}/[110]_{\text{Nb}}$, and the in-plane axes are $[11-2]_{\text{Cu}}/[1-12]_{\text{Nb}}$ and $[1-10]_{\text{Cu}}/[-111]_{\text{Nb}}$.

FIG. 2 (color online). Snapshots of (a) Cu2.5nm/Nb2.5nm, (b) Cu5nm/Nb5nm, (c) Cu10nm/Nb10nm, (d) Cu20nm/Nb20nm multilayer models and (e) bulk Nb taken at nearly the Hugniot elastic limit (HEL). The atoms are colored by common neighbor analysis (CNA). Note that the partial dislocations are emitted from the interfaces into the Cu layers for (a), (b) and (c), while into the Nb layers for (d) and (e).

FIG. 3 (color online). Snapshots of (a) Cu2.5nm/Nb2.5nm, (b) Cu5nm/Nb5nm, (c) Cu10nm/Nb10nm, (d) Cu20nm/Nb20nm multilayers with a KS orientation relationship at time = 19.5 ps (near the end of shock compression). In each panel, the sample is travelling at a particle velocity $u_p=650$ m/s. The atoms are colored according to their common neighbor analysis (CNA). The deformation in Cu is mediated by Shockley partials and in Nb by $\{110\}\langle 111 \rangle$ slip.

FIG. 4 (color online). a) Side view and b) top view of dislocation nucleation from a misfit dislocation lines within the interface into the Cu crystal at timestep = 6.5 ps and c) side view and d) top view of the dislocation transmission from the Cu side into the Nb side at the timestep of 7ps, along the misfit dislocation line. The sample is travelling upward at a particle velocity $u_p=650$ m/s towards a stationary piston at the top, which specularly reflects any particles that reach it; a resulting shockwave travels downward.

FIG. 5 (color online). Schematic showing slip system transmission from a top layer/grain into the adjacent bottom layer/grain. The slip plane normal of the top and bottom layers are n and

n' , respectively and the Burgers vectors are b and b' , respectively. The *geometric compatibility factor* is defined as $m' = \cos \varphi \cos \lambda$, where φ is the angle between the slip direction, i.e. $\text{angle}(b, b')$, and λ is the angle between the normal to the slip planes, i.e. $\text{angle}(n, n')$.

FIG. 6 (color online). (a) Orientation of the fcc and bcc gliding planes with respect to the KS interface to indicate the most probable transmission pathway. (b) Top view of the atomic structure from the Cu side together with the traces of the gliding planes at the interface, black ABC' is for the Nb side, pink ABC for the Cu side. The interface normal is assigned as $[111]_{\text{Cu}}/[110]_{\text{Nb}}$ with $[11-2]_{\text{Cu}}/[1-12]_{\text{Nb}}$ and $[1-10]_{\text{Cu}}/[-111]_{\text{Nb}}$. The transmission paths from Cu to Nb (or from Nb to Cu) are $ABD_{\text{Cu}} \rightarrow A'B'E'_{\text{Nb}}$, $BCD_{\text{Cu}} \rightarrow B'C'F'_{\text{Nb}}$, $ACD_{\text{Cu}} \rightarrow A'C'G'_{\text{Nb}}$. The possible slip systems are shown in Fig. 1c and 1d.

FIG. 7 (color online). a) Side view and b) bottom view of dislocation transmission from Cu into Nb at 8ps and c) side view and d) top view of dislocation transmission from Nb into Cu at 8.5ps. The sample is travelling upward at a particle velocity $\mu_p = 650$ m/s towards a stationary piston at the top, which specularly reflects any particles that reach it; a resulting shockwave travels downward.

FIG. 8 (color online). The change in the atomic structure of the Cu/Nb interface during dislocation transmission from the Cu side to the Nb side at a timestep of 8 ps (see Fig. 3a) (a) top view from Cu side and (b) bottom view from Nb side. The interface normal is $[111]_{\text{Cu}}/[110]_{\text{Nb}}$.

FIG. 9 (color online). Change in atomic percent of the central symmetry factor (CSF) for values of CSF greater than unity for the Cu 5nm/Nb 5nm multilayer model. The annealing times indicate dislocation recovery processes upon shock release.