LA-UR- 06-7893

*Approved for public release;*
*distribution is unlimited.*

| | |
|---|---|
| *Title:* | Room-Temperature Dislocation Climb in Copper-Niobium Interfaces |
| *Author(s):* | Jian Wang, Richard G. Hoagland, John P Hirth, and Amit Misra |
| *Intended for:* | Physical Review Letters |

Los Alamos
NATIONAL LABORATORY
EST. 1943



Form 836 (7/06)

**Room-Temperature Dislocation Climb in Copper-Niobium Interfaces**

Jian Wang[1], Richard G. Hoagland, John P Hirth*, and Amit Misra*
Materials Science and Technology Division,
* Center for Integrated Nanotechnologies, Materials Physics and Applications Division,
Los Alamos National Laboratory, Los Alamos, NM 87545, USA

## ABSTRACT

Using atomistic simulations, we show that dislocations climb efficiently in metallic copper-niobium interfaces through absorption and emission of vacancies in the dislocation core, as well as an associated counter diffusion of Cu atoms in the interfacial plane. The high efficiency of dislocation climb in the interface is ascribed to the high vacancy concentration of 0.05 in the interfacial plane, the low formation energy of 0.12 eV with respect to removal or insertion of Cu atoms, as well as the low kinetic barrier of 0.10 eV for vacancy migration in the interfacial Cu plane. Dislocation climb in the interface facilitates reactions of interfacial dislocations, and enables interfaces to be in the equilibrium state with respect to concentrations of point defects.

[1] Corresponding Author: Dr. Jian Wang, E-mail: wangj6@lanl.gov, Phone: 1-505-667-1238

Interfaces between dissimilar metals often exhibit unique atomic arrangements and properties that are not found in bulk crystals [1-7]. For example, Cu-Nb interfaces exhibit multiple atomic structures with nearly degenerate energies [8-13]. These interfaces act as sinks for vacancies and interstitials and enhance their recombination, allowing Cu-Nb nanolayered composites to persist in a damage-free steady state even when driven out of equilibrium by intense particle radiation [13,14]. With regard to mechanical properties, the blockage of slip by interfaces leads to high flow strengths in nanoscale multilayered composites [8-12]. The role of interfaces in slip transmission becomes particularly important when the individual layer thickness is less than approximately 5 nm, since dislocation pile-ups cannot form and crossing of individual dislocations across interfaces becomes the critical unit process [4-6].

Atomistic simulations of the interaction of glide dislocations with Cu-Nb reveal that these interfaces act as strong barriers for slip transmission because the dislocation core spreads in interfaces as a result of their low shear resistance [8-12]. These simulations were performed at 0K under an applied shear stress. These results imply that a dislocation with a spread core in the interface plane is strongly pinned. An important question raised is: how does a dislocation with its core spread in the interface plane cross the interface? One possible mechanism is that the spread core may reassemble at finite temperatures, e.g., via climb, thereby facilitating slip transmission [14, 15].

In this letter, we report on molecular dynamics simulations that explore the interaction of a glide dislocation with Cu-Nb interface at 300 K with no applied stress. The interaction of a discrete (3 dislocations) pile-up with the interface at 300 K is also studied with a stress applied to counter the back stress of the pile-up. The phenomenon of

dislocation climb in interfaces and related properties, such as formation energy and migration kinetics of vacancies in interfaces are discussed. Finally, we draw conclusions based on molecular dynamics simulations and theoretical estimation.

Using atomistic modeling, we assemble a bilayer model composed of two semi-infinite perfect crystals of Cu and Nb with the experimentally observed Kurdjumov-Sachs (KS) epitaxial orientation relation, corresponding to $\{111\}_{Cu}\|\{110\}_{Nb}\|$interface-plane and $<110>_{Cu}\|<111>_{Nb}$ in the interface plane, and is fully relaxed at 300K [8-12]. The coordinate system adopted is: x-axis along $[11\bar{2}]_{Cu}$ parallel to $[1\,\bar{1}2]_{Nb}$, y-axis along $[111]_{Cu}$ parallel to $[110]_{Nb}$, and z-axis along $[1\,\bar{1}0]_{Cu}$ parallel to $[\bar{1}11]_{Nb}$. The model is periodic along the z-axis. Embedded atom method (EAM) potentials are used for Cu [17] and Nb [18]. These potentials have produced good results for surface diffusion and defect formation energies [19, 20], atomic structures and mechanical properties of the Cu-Nb interface [7-15], and the growth mechanism of Cu-Nb layered composites during physical vapor deposition [16].

A mixed dislocation $\boldsymbol{b}_1$ with Burgers vector $\frac{1}{2}\boldsymbol{a}_{Nb}\mathbf{[111]}$ gliding on Nb $\mathbf{(01\bar{1})}$ is introduced in Nb crystal of the bilayer model (Fig. 1a) by the application of the anisotropic Barnett-Lothe solutions [21] for the displacement field of a dislocation on an interface between two elastically dissimilar materials. The dislocation line is parallel to the z-axis, initially situated at a distance of 1.5 nm from the interface. Molecular dynamics simulations are carried out for 120 ps at a constant temperature of 300 K. The dislocation spontaneously enters the interface at zero applied stress. The schematized process of the interaction of the dislocation with the interface is shown in Fig 1 (a) and (b), and atomic structures in Fig 1 (c) and (d) after the dislocation enters the interface.

Very importantly, the dislocation $\boldsymbol{b}_1$ dissociates into an interfacial dislocation $\boldsymbol{b}_2$ through the transport of vacancies and Cu atoms within the interface. As a consequence, an interfacial discontinuity $\boldsymbol{b}_3$ is left near the trace of the Nb slip (Fig. 1 b and c). The out-of-plane component of Burgers vector of the dislocation $\boldsymbol{b}_2$ is 0.2087 nm that is equal to the spacing of Cu {111} plane, $\frac{1}{3}\boldsymbol{a}_{Cu}[\mathbf{111}]$. On the basis of the conservation law of dislocations, the out-of-plane component of the interfacial discontinuity $\boldsymbol{b}_3$ is 0.0247 nm. Since dislocation cores readily spread within the interface [8-12], it is hard to quantify the in-plane components of Burgers vectors of the interfacial dislocation and the interfacial discontinuity, respectively.

This dissociation process is energetically favorable due to the reduction of line energies of dislocations, $\boldsymbol{b}_1^2 > \boldsymbol{b}_2^2 + \boldsymbol{b}_3^2$, according to the approximate Frank rule [22]. This process can be explained in terms of dislocation climb mechanisms. When the dislocation enters the interface, it acts as a source for vacancies, emitting vacancies; the interfacial Cu plane acts as a sink for vacancies, absorbing vacancies accompanied with a counter diffusion of Cu atoms in the interface to the dislocation core, as shown in Fig. 1c. Consequently, a patch of extra Cu (111) forms at the end of the half plane of Nb (110). Fig. 1d shows the atomic structure of the interfacial Cu plane. The change of areal density of Cu atoms in the interfacial Cu plane, from 17.74 atoms/nm$^2$ to 16.80 atoms/nm$^2$, clearly indicates the absorption of vacancies in the interfacial Cu plane and the counter diffusion of Cu atoms from the interfacial Cu plane to the dislocation core. Through emission of vacancies and absorption of Cu atoms at the dislocation core, the out-of-plane component of dislocation $\boldsymbol{b}_1$ dissociates into two parts, one part $\boldsymbol{b}_2$ moving

within the interface by climb.

In a different atomistic simulation, a dislocation pile-up in Cu crystal is blunted through climb into the interface plane. The schematized process of the pile-up blunting in the interface is shown in Fig. 2 a-c, and atomic structures in Fig. 2 d and e after a three-dislocation pile-up in Cu crystal enters the interface at an applied tensile stress of $\sigma_{xx}$ = 2.5 GPa. Initially, 3 identical mixed dislocations with Burgers vector $\frac{1}{2}\boldsymbol{a}_{Cu}[\mathbf{011}]$ pile up on glide plane Cu $(\mathbf{11\bar{1}})$ (Fig. 2a) that are introduced by the application of the anisotropic Barnett-Lothe solutions [21] for the displacement field of a dislocation on an interface between two elastically dissimilar materials; the first two dislocations $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$ enter the interface under the applied tensile stress (Fig. 2b); then they are separated by climb in the interface to reduce the line energy (Fig. 2c). Molecular dynamics simulations are carried out for 120 ps at a constant temperature of 300 K. The local atomic structure of dislocations at the climbing region shows the blunting and spreading of the 3-dislocation pile-up in Fig. 2d. The blunting and spreading process of the 3-dislocation pile-up in the interface is energetically favorable due to the associated large decrease in the line energy $(3\boldsymbol{b})^2 > 3\boldsymbol{b}^2$. This process can be explained in terms of dislocation climb mechanisms. The dislocation $\boldsymbol{b}_1$ climbs through absorption of vacancies, but $\boldsymbol{b}_2$ through emission of vacancies, both associated with a counter diffusion of Cu atoms in the interface. Transport of vacancies and Cu atoms in the interface is shown in Fig. 2 c and d with the red arrows denoting the diffusion of vacancies and the black arrows indicating the diffusion of Cu atoms. Since the first two dislocations climb in the interface away from the trace of the Cu slip, the dislocation $\boldsymbol{b}_3$ enters the interface. Two Shockley partial

dislocations dissociated from the dislocation are the leading partial $\boldsymbol{b}_3^L$ ($\frac{1}{6}\boldsymbol{a}_{Cu}[\mathbf{112}]$) and the trialing partial $\boldsymbol{b}_3^T$ ($\frac{1}{6}\boldsymbol{a}_{Cu}[\bar{\mathbf{1}}\mathbf{21}]$) that are connected by a stacking fault (marked as a red solid line). Fig.2e depicts the atomic structure of the interfacial Cu plane. The areal density of Cu atoms in the interfacial Cu plane decreases from 17.74 atoms/nm$^2$ to 17.00 atoms/nm$^2$, revealing adsorption of vacancies in the interfacial Cu plane and the counter diffusion of Cu atoms in the interfacial Cu plane. In addition, Cu atoms (red spheres in Fig. 2e) initially situate in the right side of the dislocation $\boldsymbol{b}_3^L$, between the dislocation $\boldsymbol{b}_3^L$ and the dislocation $\boldsymbol{b}_1$, then diffuse into the left side of the dislocation $\boldsymbol{b}_3^L$, between the dislocation $\boldsymbol{b}_3^L$ and the dislocation $\boldsymbol{b}_2$. This transportation of Cu atoms reveals the absorption mechanism of vacancies with respect to the climb of the dislocation $\boldsymbol{b}_1$, and the emission mechanism of vacancies with respect to the climb of the dislocation $\boldsymbol{b}_2$. As a consequence, the three dislocations from the pile-up are widely spread in the interface.

The dislocation climb observed in our simulations involves only diffusion of Cu atoms in the interfacial Cu plane: the diffusion of Nb atoms in the interface or of either Cu or Nb in the bulk crystals is negligible. This occurs because an atomic arrangement with an interfacial Nb vacancy lowers its energy by exchanging with an interfacial Cu atom thereby creating a Cu vacancy [9, 13]. In addition, there is a huge difference in the formation energies of vacancies in Cu and Nb crystals (>1.2 eV/atom) compared to vacancy formation within the interface (< 0.15 eV/atom) [9, 14, 15].

The rate of climb depends on the vacancy concentration and vacancy diffusivity in the interface. In general, climb motion is rarely observed in atomistic simulations, because the simulation period is short (less than a nano-second), and because crystalline

materials have a relatively low vacancy concentration, a high vacancy migration energy and a high vacancy formation energy [23]. The dislocation climb observed in the Cu/Nb interface implies that the Cu/Nb interface has a high vacancy concentration and a high diffusivity of vacancies. Atomistic Monte Carlo simulations indicate that the interface has the very high vacancy concentration of 0.05, about 14 orders of magnitude higher than the vacancy concentration in the bulk Cu crystal [13]. The diffusivity of such a vacancy depends on its formation and migration energies in the interfacial plane. Atomistic simulations show that a point defect in the Cu-Nb interface spreads and delocalizes within the interface instead of being locating at a crystal site [9, 13]. As a consequence, the migration of vacancies in the interfacial plane is not localized at a single atom site as in the case of bulk crystals, but rather is spread over a group of atoms. The mean extended vacancy formation $E_f$ with respect to removal of atoms in the interfacial Cu layer is computed to be 0.12 eV/atom [13]. This formation energy is one order of magnitude smaller than the formation energies of vacancies (1.26 eV) or interstitials (3.24 eV) in bulk Cu. In addition, the migration of a point defect in the interfacial plane involves the rearrangement of a group of atoms with an associated delocalized displacement field within the interface, unlike single atom jumps for a vacancy in a bulk crystal. Using the Nudged Elastic Band method, we compute the kinetic barriers associated with the migration from one delocalized displacement field to the other by molecular statics simulations. The barriers are in the range of 0.03 to 0.10 eV, since the delocalized extent of a "vacancy" within the interface varies with respect to the position of a removal of Cu atom within the interfaces. This small kinetic barrier is comparable

with a Cu adatom diffusing on a flat Cu (111) surface [19, 20], and results in the high diffusivity of vacancies within interfaces.

Molecular dynamics simulations indicate that dislocation climb in the interface is very efficient. With respect to the simulation case shown in Fig. 1, we now estimate the climb velocity. Two different processes are considered: (1) the process of vacancy emission or absorption in the dislocation core, and (2) the long-range vacancy diffusion process that accompanies the climb motion [24-28]. We limit our attention to the case that the dislocation acts as a perfect source for vacancies, and the interface acts as a sink for vacancies. Since the vacancy emission process is rapid compared to the long-range transport of vacancies, local quasi-equilibrium is assumed for vacancies at the dislocation core, providing a boundary condition [26-28].

Vacancy diffusion occurs in a one-dimensional vacancy concentration gradient, along x-axis direction, perpendicular to the dislocation line in the interfacial plane. The net rate of increase of vacancy concentration in an element $dx$ at a position $x$ consists of two parts, the net flow into the element and the generation within the element. The net flow of vacancy into the element $dx$ is $\left[\frac{dc}{dx}(D_v\frac{dc}{dx})\right]dx$ from both sides. $D_v$ is the vacancy diffusion coefficient, and $dc/dx$ the vacancy concentration gradient. On the other hand, the generation rate of vacancies in the element is $C^g(x,t)dx$. $C^g(x,t)$ is the generation rate of vacancies at position $x$.

The climb distance $h$ of the dislocation during a short period $\delta t$ is a linear function of the climb velocity, $h = v_d(t)\delta t$, where $v_d(t)$ is the climb velocity of the dislocation. The number of the emitted vacancies from the dislocation in the period $\delta$t is

$$I_v = \frac{hb}{\Omega_a} = \frac{bv_d(t)\delta t}{\Omega_a} \tag{1}$$

where $\Omega_a$ is atomic volume, and $b$ is the magnitude of the Burgers vector of the climbing dislocation. Since the local quasi-equilibrium is assumed for vacancies at the dislocation, the generation rate of vacancies is same as the emission rate of vacancies at the dislocation core. From Eq.1, the generation rate is derived as a function of the dislocation climb velocity, $v_d(t)$, and the dislocation location, $x_d = \int_0^t v_d(\tau)d\tau$.

$$C^g(x,t) = \frac{dI_v}{dt} = \frac{bv_d(t)}{\Omega_a}\delta(x - x_d) = \frac{bv_d(t)}{\Omega_a}\delta(x - \int_0^t v_d(\tau)d\tau) \tag{2}$$

$\delta(x - x_d)$ is the step function which defines the emission of vacancies at the dislocation core. With respect to a moving source of vacancies, Fick's second law becomes

$$\frac{\partial c}{\partial t} = D_v\frac{\partial^2 c}{\partial^2 x} + \frac{bv_d(t)}{\Omega_a}\delta[x - \int_0^t v_d(\tau)d\tau]dx \tag{3}$$

The solution of vacancy concentration for the above Eq. (3) can be found in Ref. [29] ,

$$c(x,t) = C^\infty + \frac{1}{\sqrt{2\pi D_v}}\frac{b}{\Omega_a}\int_0^t \frac{v_d(t)}{\sqrt{t-\tau}}\exp[-\frac{(x - \int_0^t v_d(\sigma)d\sigma)^2}{4D_v(t-\tau)}]d\tau \tag{4}$$

$C^\infty$ is the initial vacancy concentration in the interfacial plane. We determine the climb velocity $v_d(t)$ from Eq. (4) by satisfying the boundary condition, $c(\int_0^t v_d(\sigma)d\sigma, t) = C^{eq}$, in which vacancy concentration at the dislocation is equal to its equilibrium value.

$$v_d(t) = \frac{(C^{eq} - C^\infty)\sqrt{2\pi D_v}\Omega_a}{2b\sqrt{t}} \tag{5}$$

Replacing the climb velocity in Eq. (4) with Eq. (5), vacancy concentration in the interfacial plane can be determined.

Using Eqs. (4) and (5), we compute the distribution of vacancy concentration in the interfacial plane and the climb velocity of the dislocation with parameters: $C^{\infty} = 0$, $C^{eq} = 0.05$ , $b = 0.2087$ nm, $\Omega_a = \frac{1}{4} a_{Cu}^3$ , $D_v = D_0 \exp(-\frac{E_f^v + E_f^m}{k_B T})$ , $E_f^v = 0.12eV$ and $E_f^m = 0.1eV$ . Here $a_{Cu}$ is the lattice parameter for the Cu crystal, $k_B$ is Boltzman's constant, T is degrees K. $D_0$ is the pre-exponential factor, 0.36 $cm^2$/sec which is not expected to differ markedly for vacancy diffusion in Cu crystal [28, 30]. Fig. 3a shows the climb velocity as a function of time and temperature, and Fig. 3b shows the distribution of vacancy concentration at different times during dislocation climb. At room temperature, the climb velocity is around 0.5 m/s, about 5 orders of magnitude larger than the climb velocity in Cu crystal.

Before closing, we discuss the importance of dislocation climb. Through climb, the out-plane component of interfacial dislocations can move within the interface, react with other interfacial dislocations, and interact with point defects in the interface. Firstly, this climb enables slip transmission: glide dislocations can reassemble the spread cores in the interface plane via climb, and dislocation debris scattered in interfaces can reassemble into lattice glide dislocations, facilitating slip transmission. Secondly, reactions between interfacial dislocations assisted by climb could lead to annihilation of dislocation content (recovery). Thirdly, discrete pile-ups can be absorbed in the interface plane, assisted by climb in the interface, thereby blunting the stress concentration of the pile-up. This implies that unless a long pile-up can form, the slip transmission across Cu-Nb interfaces will not be assisted by the mechanical advantage of the pile-up. Thus, in nanolayered materials where long pile-ups cannot form, crossing of single dislocations across the

interface is the critical unit process and may be assisted by climb in the interface. Finally, dislocation climb enables the interfacial plane to be in an equilibrium state with respect to concentrations of point defects because of absorption and/or emission of vacancies at dislocation cores. Thus, these interfaces act as ideal sinks for vacancies and interstitials, allowing Cu-Nb nanolayered composites to persist in a damage-free steady state even when driven out of equilibrium by intense particle radiation.

In summary, this letter reports that dislocations climb in Cu-Nb interfaces at room temperature. Using atomistic modeling and theoretical analysis, we show that dislocations climb efficiently through absorption and emission of vacancies in the dislocation core, as well as an associated counter diffusion of Cu atoms in the interfacial plane. The high efficiency is ascribed to the high vacancy concentration of 0.05 in the interfacial plane, the low formation energy of 0.12 eV with respect to removal or insertion of Cu atoms, as well as the low kinetic barrier of 0.10 eV for vacancy migration in the interfacial Cu plane. Dislocation climb in the interface facilitates reactions of interfacial dislocations, and enables interfaces to be in the equilibrium state with respect to concentrations of point defects.

**Acknowledgements:** This work was supported by the US Department of Energy, Office of Basic Energy Sciences.

**References**

1. Misra A, Verdier A, Lu YC, Kung H, Mitchell TE, Nastasi M, and Embury JD, Scrip. Mater 1998; 39: 555
2. Clemens BM, Kung H, and Barnett SA, MRS Bull 1999; 24: 20
3. Phillips MA, Clemens BM, and Nix WD, Acta Mater 2003; 51: 3157
4. Misra A, Hoagland RG, and Kung H, Phil. Mag. 2004; 84: 1021
5. Misra A, Hirth JP, Hoagland RG, Embury JD, and Kung H, Acta Mater 2004; 52:

2387

6. Misra A, Hirth JP, and Hoagland RG, Acta Mater 2005; 53: 4817
7. Hoagland RG, Kurtz RJ, and Henager CH, Scrip. Mater 2004; 50: 775
8. Hoagland RG, Hirth JP, and Misra A, Phil. Mag. 2006; 86: 3537
9. Demkowicz MJ, Wang J, and Hoagland RG, in J. P. Hirth (Ed.), *Dislocations in Solids,* Vol. 14, Chap. 83. Elsevier, North-Holland, 2008, p.141
10. Wang J, Hoagland RG, Hirth JP, and Misra A, Acta Mater 2008; 56: 3109
11. Misra A, Demkowicz MJ, Wang J, and Hoagland RG, JOM 2008, April: 39
12. Wang J, Hoagland RG, Hirth JP, and Misra A, Acta Mater 2008; 56: 5685
13. Demkowicz MJ, Hoagland RG, and Hirth JP, Phys. Rev. Lett. 100:136102 (2008)
14. P. M. Derlet, P. Gumbsch, R. G. Hoagland, J. Li, D. L. McDowel, H. Van Swygenhoven, and J. Wang, MRS Bulletin, March (2009).
15. Wang J, Hoagland RG, and Misra A, Scripta Mater. (2009).
16. Wang J, Hoagland RG, and Misra A, J. Mater. Res. 2008; 23: 1009
17. Voter AF and Chen SP, Mater. Res. Soc. Symp. Proc. 1987; 82: 175
18. Johnson RA and Oh DJ, J. Mater. Res. 1989; 4: 1195
19. Huang H and Wang J, Appl. Phys. Lett. 2003; 83: 4752
20. Wang J, Huang H, and Cale TS, Model. Simul. Mater. Sci. Eng. 2004; 12: 1209
21. Barnett DM and Lothe J, J. Phys. F 1974; 4: 1618
22. Hirth JP and Lothe J, Theory of Dislocations, 2nd edn. Krieger, Melbourne FL, chap 22, 1992
23. Shewmon P, Diffusion in Solids, McGraw-Hill Book Co., New York (1963).
24. Balluffi RW, Phys. Stat. Sol. 31: 443, 1969
25. Thompson D.O., Buck O, and Huntington HB, J. Appl. Phys. 38: 3057, 1967
26. Lothe J, J. Appl. Phys.31:1077, 1960
27. Nix WD, Gasca-Neri R, and Hirth JP, Phil. Mag. 23: 1339, 1971
28. Seidman DN and Balluffi RW, Phil . Mag., 13:649-654, 1966
29. Sneddon Ian N., Fourier Transforms, McGraw-Hill Book Co., New York (1951) p. 193-200
30. Gupta D, Diffusion in Bulk solids and Thin Films, in Diffusion Processes in Advanced Technological Materials, p50, edited by D. Gupta, William Andrew Publishing, Norwich, NY, USA, 2005

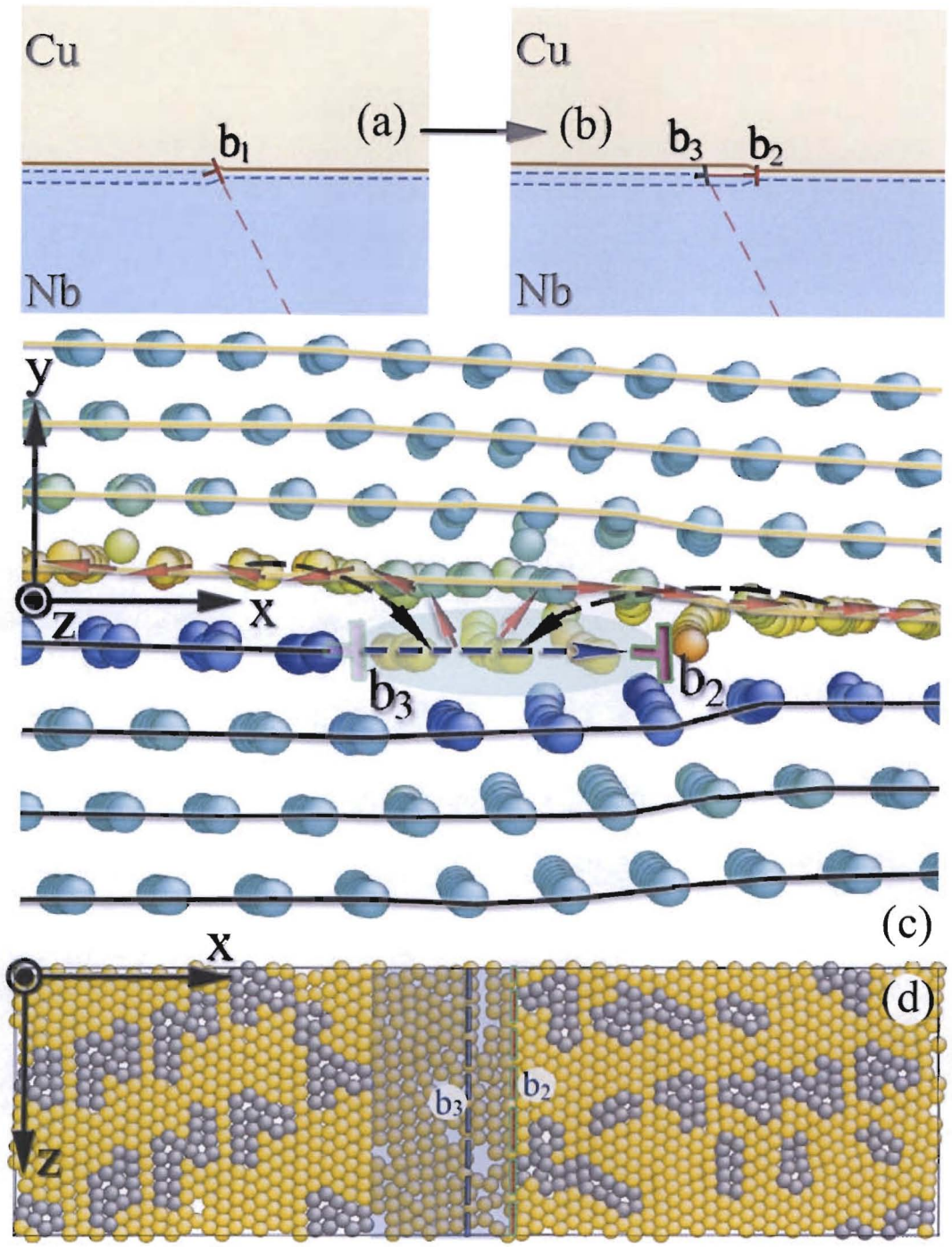
**Figure Captions**:

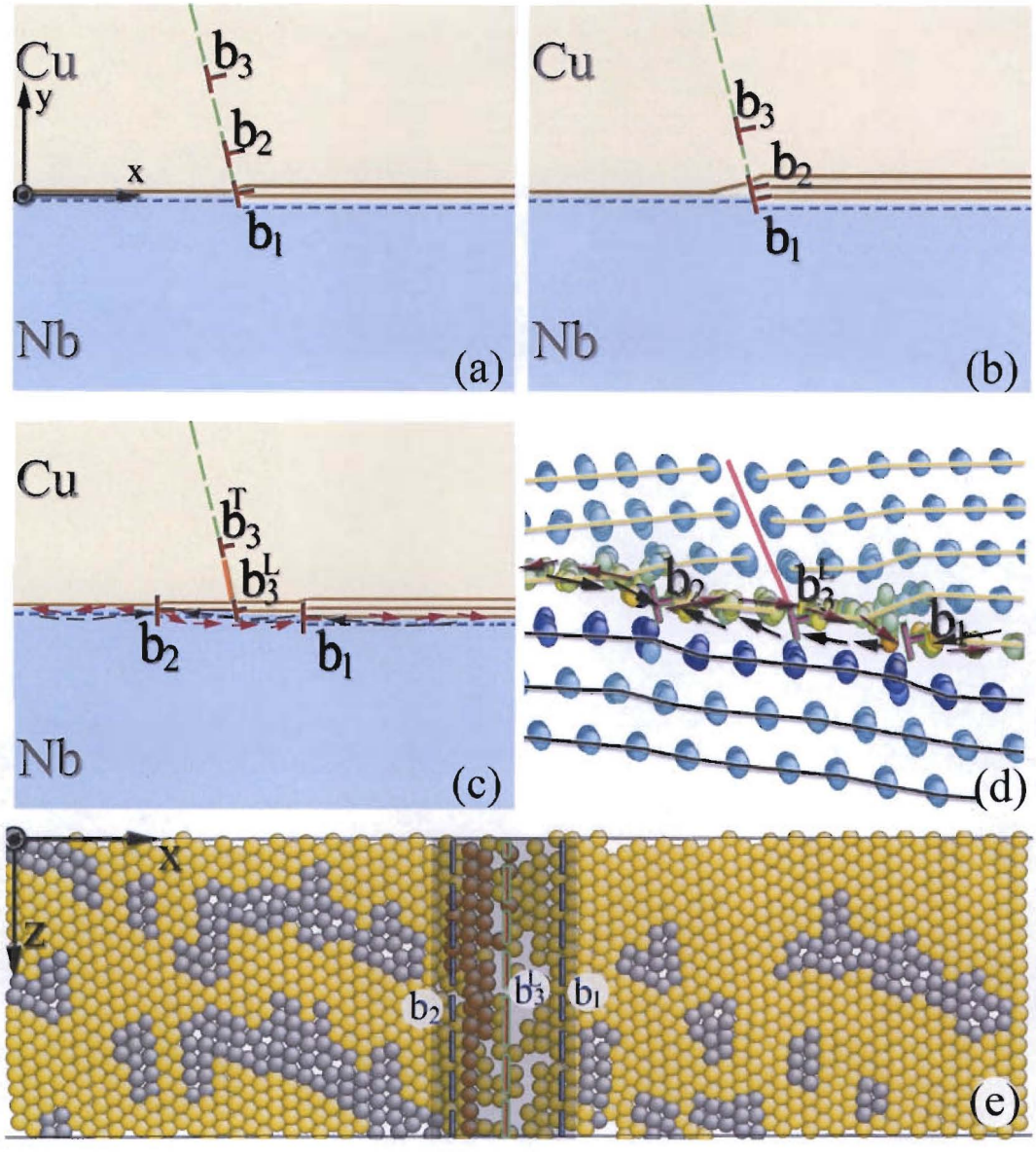
Figure 1: The dissociation of a mixed dislocation $b_1$ ($\frac{1}{2}\boldsymbol{a}_{Nb}[111]$) in the Cu/Nb interface through dislocation climb. The schematic plots show (a) a mixed dislocation $b_1$ situated at the interface and (b) the dissociation of the dislocation into an interfacial dislocation $b_2$ ($\frac{1}{3}\boldsymbol{a}_{Cu}[111]$) through transportation of vacancies and Cu atoms within the interfacial Cu plane, and an interfacial discontinuity $b_3$ ($\frac{1}{2}\boldsymbol{a}_{Nb}[111]$-$\frac{1}{3}\boldsymbol{a}_{Cu}[111]$) left near the trace of the Nb slip; (c) atomic structures after the dissociation of the dislocation $b_1$ in the interface. The red arrows indicate the diffusion of vacancies and the black arrows indicate the counter diffusion of Cu atoms. Atoms in (c) are colored by their excess potential energy. The yellow lines represent Cu (111) planes, and the black lines Nb (110) planes. (d) Atomic structures of the interfacial Cu plane. The dashed lines indicate locations of the two dislocations. The decrease of areal density of Cu atoms in the interfacial Cu plane reveals adsorption of vacancies and the counter diffusion of Cu atoms in the interfacial Cu plane. The regions with low areal density of Cu atoms are outlined in gray atoms and the gray shadow, and the regions with the areal density same as Cu (111) are outlined in yellow atoms.

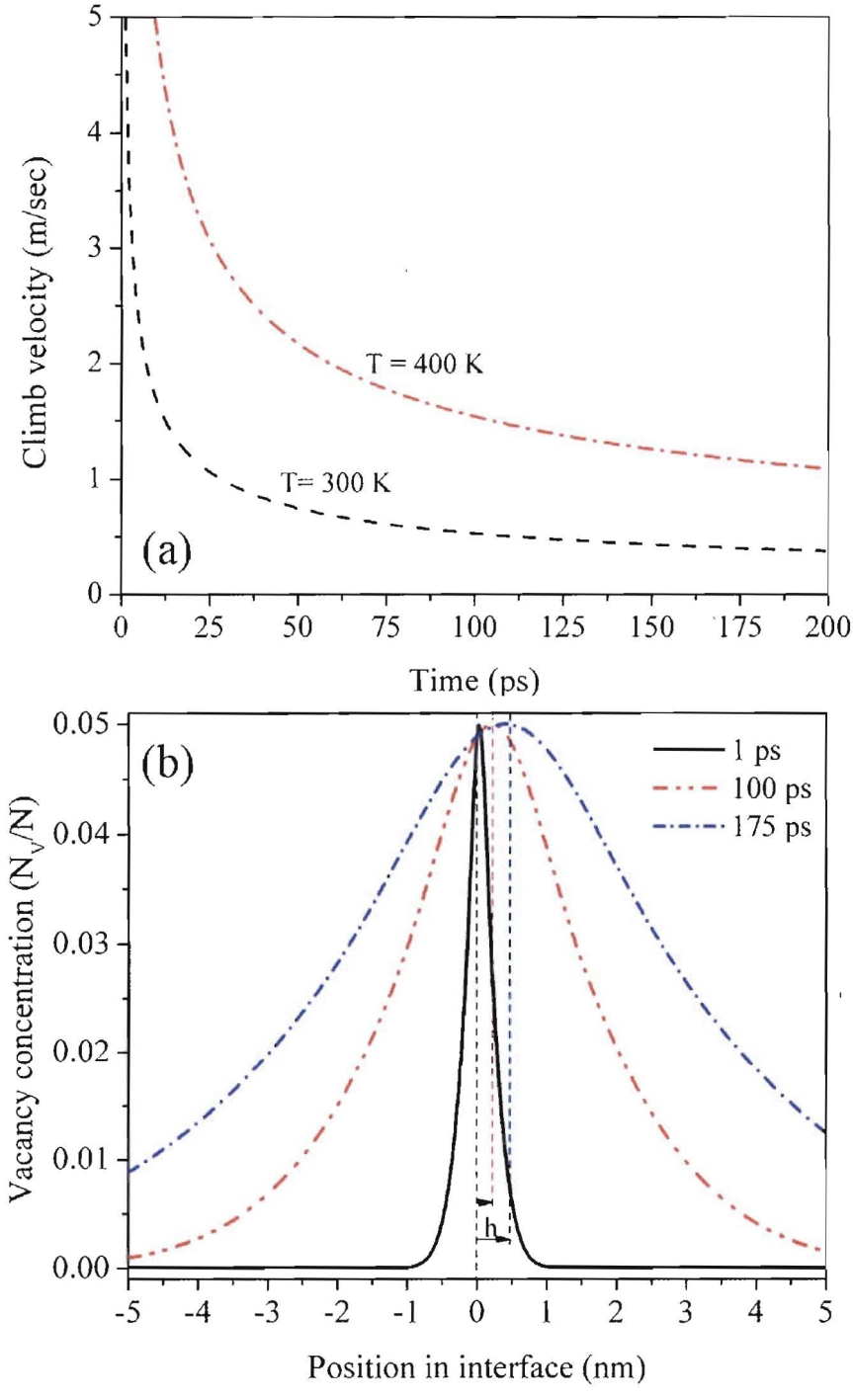
Figure 2: Absorption and spreading of a 3-dislocation pile-up at the Cu/Nb interface. The schematic plots show (a) three dislocations, $b_1$, $b_2$, and $b_3$ ($\frac{1}{2}\boldsymbol{a}_{Cu}[011]$) are initially piled up in the Cu layer, (b) the first two dislocations enter the interface under the applied tensile stress, and (c) dislocations $b_1$ and $b_2$ climb in the interface. The dislocation $b_1$ climbs through absorption of vacancies, but $b_2$ through emission of vacancies, both associated with a counter diffusion of Cu atoms. The dislocation $b_3$ dissociates into two Shockley partial dislocations: the leading partial $\boldsymbol{b}_3^L$ ($\frac{1}{6}\boldsymbol{a}_{Cu}[112]$) and the trialing partial $\boldsymbol{b}_3^T$ ($\frac{1}{6}\boldsymbol{a}_{Cu}[\bar{1}21]$), that are connected by a stacking fault marked as a red solid line. The yellow solid lines represent Cu (111) planes, and the dashed black lines Nb (110) planes in (a), (b), and (c). (d) The local atomic structure of dislocations at the climbing region. The red arrows indicate the diffusion of vacancies and the black arrows indicate the diffusion of Cu atoms. Atoms in (d) are colored by their excess potential energy. The yellow lines represent Cu (111) planes, and the black lines Nb (110) planes. (e) Atomic structure of the interfacial Cu plane. The dashed lines indicate locations of the three dislocations. Red spheres represent Cu atoms that are initially in the right of the

dislocation $\boldsymbol{b}_3^L$ and then diffuse into the left side of the dislocation $\boldsymbol{b}_3^L$, revealing absorption mechanism of vacancies with respect to the climb of dislocation $b_1$, and emission mechanism of vacancies with respect to the climb of dislocation $b_2$. In addition, the decrease of areal density of Cu atoms in the interfacial Cu plane reveals adsorption of vacancies and a counter diffusion of Cu atoms in the interfacial Cu plane. The regions with low areal density of Cu atoms are outlined in gray atoms and the gray shadow, and the regions with the areal density same as Cu (111) are outlined in yellow atoms.

Figure 3: Climb velocities of interfacial dislocations and distribution of vacancy concentration in the interface. (a) Dependence of the climb velocity on temperature and time, and (b) vacancy concentration in the interface at different instants during dislocation climbing at room temperature. The dashed lines indicate the location of the dislocation at different instants, and $\boldsymbol{h}$ the climb distance of the dislocation


Cu
Nb
(a)
b1
Cu
Nb
(b)
b3
b2
y
x
z
b3
b2
(c)
x
z
b3
b2
(d)


Cu
y
x
b3
b2
b1
Nb
(a)
Cu
b3
b2
b1
Nb
(b)
Cu
b3T
b3L
b2
b1
Nb
(c)
b2
b3L
b1
(d)
x
z
b2
b3L
b1
(e)


Climb velocity (m/sec)
T = 400 K
T= 300 K
(a)
Time (ps)
(b)
1 ps
100 ps
175 ps
h
Vacancy concentration (N_v/N)
Position in interface (nm)