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# The role of interface in uniaxial tensile process of nano-scale bilayer Cu/Ni

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ABSTRACT

Uniaxial tensile processes of nano-scale bilayer Cu/Ni with coherent interface (CI) and semi-coherent interface (SCI) are simulated by molecular dynamics (MD). The results show that in the deformation processes of two kind of Cu/Ni bilayer structures, dislocations nucleate from interface and the leading dislocations slipping cross the interface cause the bilayer structures getting into plastic deformation stage. The SCI leads to the strength and strain rate sensitivity (SRS) depending on the thickness of the nano-scale bilayer Cu/Ni, because of SCI hindering the dislocations slipping. However, due to the weak barriers of CI, the dislocation can cross the interface easily, which cause the independent of strength and SRS values on thickness.



## 1. Introduction

As a hot topic, metallic nano-scale bilayer films are potential materials for technological applications and fundamental scientific research [1]. In these nano-composites, the heterogeneous internal interfaces play a dominant role in determining the deformation and strengthen mechanisms [2–4]. There are three mechanisms depend on the thickness of layer between the neighbor two interfaces [5–8]: (1) As the layer thickness is greater than the range of tens to hundreds nanometers, strength dependents on the length scale of the material via the H-P model which is came from the dislocations pileup at the interfaces; (2) in the few to a few tens of nanometers range, strength increases with decreasing layer thickness, which can be interpreted as confined layer slip model; (3) as the layer thickness decreases below the typical dislocation core dimensions, the dislocation nucleation mechanism govern the deformation behavior which is influenced by coherent stresses, misfit dislocations, elastic moduli mismatch and the chemical mismatch [9,10].

The parameters of the function describing the size effect on strength are varying according to the strain rate [11–13]. Many efforts have been paid to investigate the size effect of layer thickness on SRS [11–15]. For nano-crystalline or nano-twinned metals, the twin boundaries and grain boundaries play an increasingly important role in determining the mechanical properties of materials, which causes the increasing SRS with decreasing feature size [11–13]. Zhang et.al. [14,15] reported that the monotonic increase in SRS of nano-crystalline Cu/X (X = Cr, Zr) nanolayers with reducing layer thickness is caused due to more dislocation-interface interactions, while the non-monotonic behavior of nano-twinned Cu/X (X = Cr, Zr) nanolayers stem from the competing effects between nano-twins and interfaces/grains on SRS.

In the nano-scale size, as the interface varies from coherent to incoherent structure, the leading dislocations slip across the interface generally presentation as continue and discontinuous fashions, respectively [10]. It can be deduced that the size effect on deformation process, strength and SRS of nano-scale bilayer structures may be distinct due to the difference of coherent stresses and misfit dislocations, etc. In the present study, MD method is employed to simulation the deformation process of nano-scale bilayer Cu/Ni with CI and SCI under uniaxial tensile. Different layer thickness and strain rate are used in the simulations to investigate the size dependence of strength and SRS of bilayer Cu/Ni.

## 2. Simulation methods

In atomistic simulation field, the embedded atom method (EAM) potential is a classical interatomic potential for describing the energy between atoms in metal alloy. In the simulation models, the interactions between atoms (Cu—Cu, Ni—Ni and Cu—Ni) are described by the EAM potential constructed by Zhou et al. [16]. The MD simulations are performed using large-scale atomic/-molecular massively parallel simulator (LAMMPS) [17]. The open

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visualization tool (OVITO) [18] with common neighbor analysis (CNA) and dislocation analysis (DXA) method is employed to analysis microstructure of models and post-processing atomic data obtained from MD.

Two types Cu/Ni bilayer models with SCI (Model-A) and CI (Model-B), as shown in Fig. 1(a) and (b), are constructed by joining Cu and Ni crystals with same crystallographic orientations and coordinates, the $x$-axis along [1 1 1], $y$-axis along [1 1 $\bar{2}$], and $z$-axis along [$\bar{1}$ 1 0]. Periodic boundary conditions are applied for three dimensions. The equivalent lattice constant being half of ($a_{Cu} + a_{Ni}$) is used to build Cu/Ni bilayer with CI. In this way, the coherency strain of Cu and Ni is $\varepsilon_{yy} = \varepsilon_{zz} \approx -0.013$ and $\varepsilon_{yy} = \varepsilon_{zz} \approx 0.013$, respectively [19]. Considering the concept of coincidence site lattice on the misfit interface [20], for minimize the internal stress of SCI, the lattice parameter number ($N \approx 37$) of Cu crystal along $y$ and $z$ is calculated by:

$$N \times a_{Cu} = (N + 1) \times a_{Ni} \quad (1)$$

where $a_{Cu}$ and $a_{Ni}$ is 0.3615 and 0.3520 nm, respectively. It indicates that within the range of misfit interphase interface, the stress induced by the difference of lattice parameters should be relaxed [21]. Then, the dimensions of the simulation cell of models with CI and SCI are chosen to be ~32.7 nm and ~18.9 nm with respect to $y$ and $z$ directions. The thickness ($\lambda$) of model is determined by number ($n$) of (1 1 1) atom layer in Cu and Ni crystal. The main model parameters of $\lambda$ and $n$ ($n = n_{Cu} = n_{Ni}$) are defined in Table 1.

All the MD simulations are performed using the Verlet integration algorithm with time step of 1.0 fs. The models are minimized energy using conjugate gradient algorithm. Then the optimized bilayer models are heating to 300 K by rate of 1.5 K/ps in an isothermal-isobaric (NPT). At last, the bilayer structures are equilibrated 50 ps in NPT ensemble for obtaining stable equilibrium system. The configurations are deformed in uniaxial tension along $y$ direction at constant strain rates (i.e. 0.1/ps, 0.025/ps, 0.05/ps and 0.01/ps) with a stress-free condition for the other two simulation cell boundaries.

**Table 1**
Thickness parameters of bilayer structures.

| Model-A | | Model-B | |
|---|---|---|---|
| $n$ | $\lambda$ (nm) | $n$ | $\lambda$ (nm) |
| 14 | 5.9 | 15 | 6.2 |
| 20 | 8.4 | 18 | 7.4 |
| 26 | 11.0 | 21 | 8.7 |
| 38 | 16.0 | 24 | 10.0 |
| 50 | 20.9 | 36 | 14.8 |
| 62 | 25.9 | 48 | 19.8 |
| 74 | 30.9 | 60 | 24.7 |
| | | 72 | 29.7 |

$n$—The (1 1 1) atom layer number of Cu or Ni; $\lambda$—the thickness of bilayer structure.

## 3. Results and discussion

### 3.1. Relaxation results

After energy minimization, as shown in Fig. 1(c), there no stacking fault (SF) exists in models with CI. Fig. 1(d) and (e) shows that the relaxed semi-coherent interface can be classified into four regions which can also be found in interface of Model-A (Fig. 1 (f)) at 300 K. In the relaxation process, the coherence of Cu and Ni increases associates with the areas of face-centered cubic (FCC) and intrinsic stacking fault (ISF) regions increase and node shrink [21,22]. At the same time, six kinds of segmental disloca-

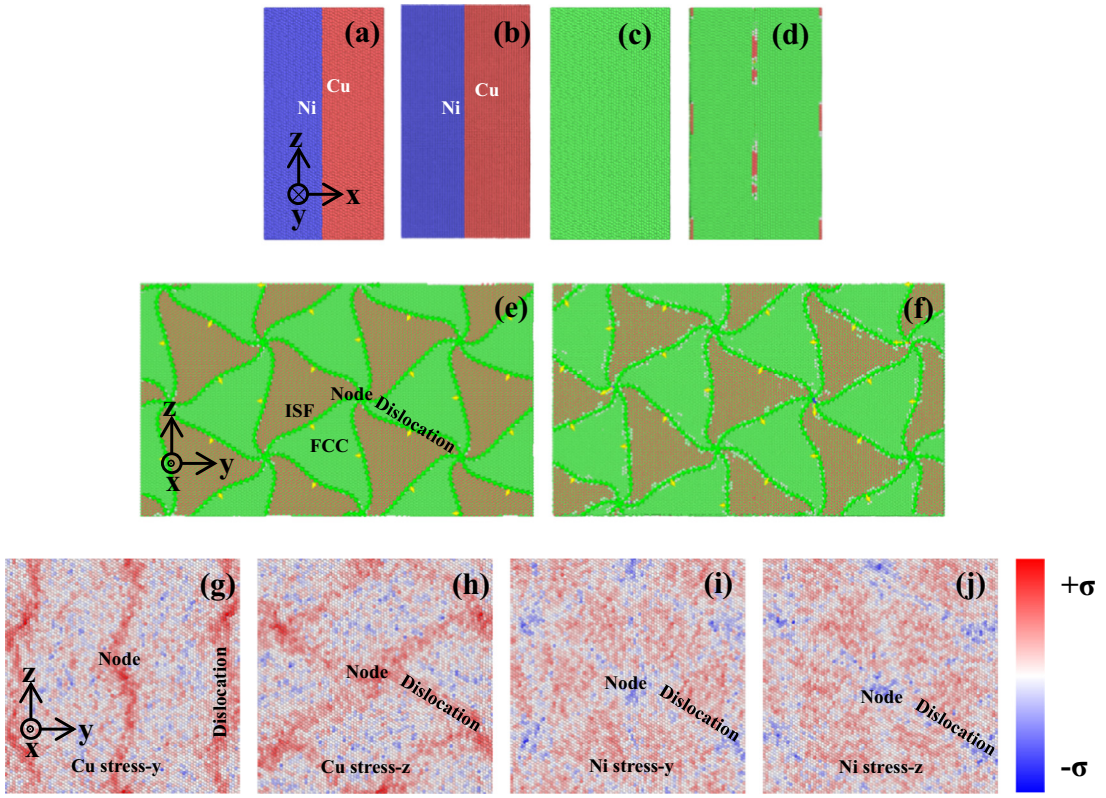


**Fig. 1.** The configurations of Cu/Ni bilayer structure with (a) CI and (b) SCI; (c) and (d) CNA analysis results; (e) and (f) DXA analysis results of SCI; (g)–(j) Stress of atoms in SCI. (Disorder, HCP and FCC atoms are labeled by white, red and green color, respectively; dislocation and Burgers vector are displayed by green and yellow line with arrow, respectively.) (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)