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Structural evolution of copper-silver bimetallic nanowires with core-shell structure revealed by molecular dynamics simulations

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ABSTRACT

The molecular dynamics simulation method is used to investigate the tensile deformation mechanism of Cu-Ag core-shell nanowires. The results for the actual structure of the Cu-Ag core-shell nanowires after energy minimization processes indicate that the atoms in shell Ag are reconstructed when the shell thicknesses smaller than 1.0 nm, while the shell thickness increases from 1.0 nm to 1.5 nm, the shape of NWs change into irregular circle. And then the tension strain is performed along the [001] direction under the conditions of varying the shell thickness and the temperature, respectively. It is found that, in low temperature region, <500 K, with decreasing the shell thickness from 1.5 nm to 0.25 nm, the plastic deformation mechanism transforms from the misfit dislocation tube mechanism into the surface dislocation nucleation mechanism. When the temperature increases to the high region, ≥500 K, the plastic deformation mechanism then changes into the high temperature influence dislocation nucleation mechanism. A shell thickness-temperature plastic deformation map is proposed to reveal the transition among the three different plastic deformation mechanisms for Cu-Ag core-shell nanowires.

1. Introduction

Metallic nanowires (NWs) are considered to be potential candidate materials for various applications in electronic, optical, catalytic and sensor industry, because of their attractive properties, such as electrical property, optical property, magnetic property and thermal property [1–6]. Especially, copper NW with high electrical conductivity and low cost is becoming one of the focused materials in microelectronics and sensors [7–9]. However, the recent investigations for the NWs show that surface oxidation severely appears when exposed it to atmosphere conditions [10,11]. Several studies indicate that silver coating with core-shell structure is the most efficient anti-oxidation way for copper NWs [7,12,13]. In recent years, the synthesis works for Cu-Ag core-shell NW have been reported by different research groups, and their results verified that the oxidation resistance ability is acquired [7,8,14].

Although the fabrication for Cu-Ag Core-shell NWs is realized, few works have been done on the role of shell thickness and operation temperature during tensile processes, which have strong influence on the mechanical and electrical properties [15–17]. In addition, the two factors compete with each other in controlling the plastic deformation in core-shell NWs [18,19]. When shell thickness and temperature are viewed as variables, two issues worth of comprehensive study are (1) what is the dominant plastic deformation mechanism in different zones? (2) how does the shell layer thickness affect the dominant plastic deformation mechanisms in core-shell NWs.

Therefore, it is important to understand the structural evolution of Cu-Ag core-shell NW during the deformation at varying shell thicknesses and temperatures, respectively. However, the experimental aimed for observing deformation behaviors of Cu-Ag core-shell NW is difficult to be carried out as it is hard to perform the various condition temperatures to observe the structures evolution and detect the microstructure transformation. Molecular dynamics (MD) simulation provides us a simple and economical way [20–23]. In 2010, Jing and his co-authors investigated the tensile deformation behaviors for Si/a-Si core-shell NWs by MD simulation, the results showed that the shell thickness has significant effects on the mechanical properties of core-shell NWs [24]. In 2012, the tensile deformation behaviors for Cu-Ag two types of sub-10 nm multilayer structures were investigated by Yuan and his partners and the results indicated that, for the structures with interfaces parallel to the structure axis, the larger total elongation for larger thickness are related to the twinning induced by plastic deformation [19]. In 2014, the strength and deformation

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mechanisms of the Cu-Ag polycrystalline metallic multilayers were studied, their results showed that grain size and layer thickness has strong influence on flow strength [25,26], and the results are consistent with high resolution TEM observation [27]. To the best of our knowledge, the study for mechanical properties and corresponding deformation mechanism in Cu-Ag core-shell NW has not been reported. Thus, MD simulation is applied to study the structural evolution in Cu-Ag core-shell NW during deformation processes with different shell thicknesses and temperatures, respectively. Furthermore, the results proposed in this paper may apply to the design process for core-shell NWs structures.

2. The simulation methods

The MD simulation is realized by the open code LAMMPS [28]. Periodic boundary condition is imposed along the wire axis z to mimic infinitely long wires, while all other directions in NWs are kept in free. The constant time step Δt is 3 fs (1 fs = 10^{-15} s). The leapfrog scheme is used for integrating the Newton's equations of motion, and the Maxwell-Boltzmann distribution is used for the initial velocities of the atoms. The circular NW with outer diameter of 8 nm consists of a single-crystalline Cu NWs covered by an Ag shell layer. The initial Cu NW with [001] is constructed first, and then the Ag layer is built on Cu NW surface with the same orientation, as shown in Fig. 1. The thicknesses of the Ag layer are 0.25 nm, 0.5 nm, 1.0 nm and 1.5 nm respectively, the detailed parameters are listed in Table 1. And this modelling approach has been successfully applied to the study for Si-Ge core-shell NWs [29]. Before the deformation processes, the NWs are subjected to energy minimization using the conjugate gradient method, then the systematic temperature gradually heated up to the desired aim in a step-wise fashion, and finally relaxed in the Nose/Hoover isobaric-isothermal ensemble (NPT) under both the pressure 0 Pa and the desired temperature (1 K, 100 K, 300 K, 500 K, 800 K and 1100 K, respectively) for 1000 ps. The NWs are

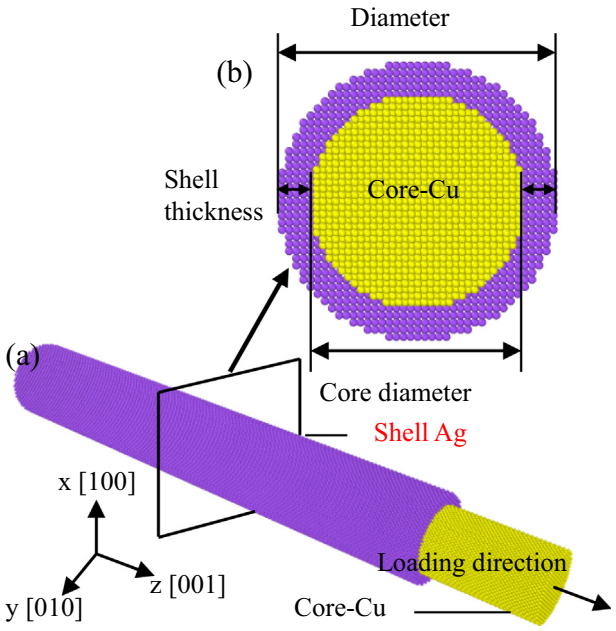

Fig. 1. The original atomic structure diagram of the Cu-Ag core-shell nanowires generated by LAMMPS, Cu atoms and Ag atoms denoted by yellow ball and purple one, respectively. (a) Perspective view depicting the [001]-oriented core shell nanowires containing core Cu and shell Ag. (b) Cross-sectional view, showing the structure schematic for core diameter, shell thickness and outer diameter.

Table 1
The parameters of different shell Ag thicknesses for Cu-Ag core-shell NWs.

Shell Ag thicknesses	Number of total atoms	The atoms number ratio between Cu and Ag
0.25 nm	250,262	1020:100
0.50 nm	238,762	506:100
1.00 nm	224,526	189:100
1.50 nm	208,926	108:100

deformed in tension by straining the simulation box at a constant deformation rate at 8×10^8 s^{-1} along the NWs axis with canonical (NVT) ensemble. On the other hand, for better understanding the influences of Ag shell structure on Cu NW, the same process is carried out for single Ag NW with the same parameters as standard sample.

The interaction between Cu-Ag atoms is described by the embedded-atom-method (EAM) potential developed by Williams et al. [30]. Generally speaking, the EAM represents the total energy of an atomic system, the expression is [31]

$$E_{tot} = \frac{1}{2}\sum_{ij} V_{ij}(r_{ij}) + \sum_i F_i(\overline{\rho}_i) \tag{1}$$

where $V_{ij}(r_{ij})$ is the pair interaction energy between atom i and j separated by a distance r_{ij}, and Fi is the embedding energy of atom i as a function of the host electron density $\overline{\rho}_i$. The latter can be written as

$$\overline{\rho}_i = \sum_{j\neq i} \rho_j(\overline{r}_{ij}) \tag{2}$$

where $\rho_j(r)$ is the electron density function assigned to atom j. For the binary Cu-Ag system used in this study, seven potential function are required: $V_{CuCu}(r)$, $V_{CuAg}(r)$, $V_{AgAg}(r)$, $\rho_{Cu}(r)$, $\rho_{Ag}(r)$, $F_{Cu}(\overline{\rho})$ and $F_{Ag}(\overline{\rho})$. Williams et al. first used an existing pure Cu EAM potential [32] to provide potential functions $V_{CuCu}(r)$, $\rho_{Cu}(r)$ and $F_{Cu}(\overline{\rho})$, and then they designed a new EAM potential for pure Ag to acquire potential functions $V_{AgAg}(r)$, $\rho_{Ag}(r)$ and $F_{Ag}(\overline{\rho})$, last, they constructed the cross-interaction function $V_{CuAg}(r)$ which is the key potential to describe interaction effect between Cu atoms and Ag atoms, the expression is given by

$$V_{CuAg}(r) = E_1[\exp(-\alpha\beta(r-r_0)) - \alpha\exp(-\beta(r-r_0)) + \delta]\psi\left(\frac{r-r_c}{h}\right) \tag{3}$$

E_1, r_0, α, β, δ, r_c and h are the Optimized values of fitting parameters, which can obtain from the first-principles data [30]. The binary Cu-Ag potential has been widely used for MD calculation [19,25–27,30,33], and the results are consistent with experimental data [27,30,33]. This indicates that the potential can accurately reproduce the behaviors for Cu-Ag core-shell NWs. In addition, OVITO is used to visualize the atomic structures [34], where atoms are colored by common neighbor analysis (CNA) [35,36]. The dislocation lines are colored by dislocation extraction algorithm (DXA) [37,38]. In addition, local atomic stresses are also calculated according to the method introduced in previous studies [39,40], and the calculation process described as follow. First, the local stress tensor σ_i on each atom i are calculated, whose components are defined as

$$\sigma_i^{ab} = \frac{1}{V_i}\sum_{j\neq i}\frac{\partial E_i}{\partial r_{ij}}\frac{r_{ij}^a r_{ij}^b}{r_{ij}} \tag{4}$$

where r_{ij}^a and r_{ij}^b (with a, b = x, y, z) are the Cartesian components of the vector r_{ij}, and r_{ij} represents modulus of vector. V_i is the atomic volume. The isotropic atomic pressure P_i is related to the trace of σ_i and the expression can be written as follow: