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Molecular dynamics simulation of Cu/Au thin films under temperature gradient

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ABSTRACT

Three modulation period thin films, 1.8 nm Cu/3.6 nm Au, 2.7 nm Cu/2.7 nm Au and 3.6 nm Cu/1.8 nm Au, are obtained from deposition method and ideal modeling based on lattice constant, to examine their structures and thermophysical characteristics under temperature gradient. The coherent lattice interface is found both at deposit and ideal thin films after annealing. Also, the vacancies are observed clearly in the deposit thin films. The defect and component of thin films will influence the energy transportation in the coatings. The vacancies and lattice mismatch can enlarge the mobility of atoms and result in the failure of coating under the thermal stress. The power spectrum of atoms' movement has no apparent rule for phonon transportation in thin films. The results are helpful to reveal the micro-mechanism and provide reasonable basis for the failure of metallic coatings.

1. Introduction

The rapid development of manufacturing and processing industry requires tool and mold materials with certain characteristics, such as super-hardness, high heat-resistance, excellent anti-wear capability, high strength, toughness and so on. Therefore, nano-multilayer coatings (NMLC) [1,2] have been proposed to meet the above requirements. This novel material promises to exhibit an extensive application in the field of aerospace, automobile, manufacture.

So far, many studies about the preparation, testing and models of NMLC have been reported [3–12]. However, many problems still need resolving before NMLC is widely used. For instance, the test criteria for the mechanical properties are different in the experiment and simulation; the formation of defect and its impacts on the properties of NMLC are unclear; the hardness mechanism and failure mechanism of NMLC need to be revealed. Besides, the temperature gradient usually exists in NMLC during the preparation and working process which will have a serious influence on its mechanical property. A deeper study of NMLC under various thermal conditions [11,13] has a great significance for the application.

It is difficult to study the properties of NMLC via conventional experimental methods due to its natural dimension. Therefore, several alternative approaches, including nano-indentation, nano-scratch, analytical model [13] and molecular dynamics (MD) simulation [14], are proposed to investigate NMLC. As a result, MD have proved to be a powerful tool in the studies of nanomaterials [15–17]. For NMLC, Landman et al. [18] tested properties of a gold surface by interacting with a nickel tip. Subsequent indentation of the gold surface caused the onset of plastic deformation of the substrate. Cheng and Lee [19] studied roughness on an aluminum coating with MD. The film surface roughness was influenced by the substrate temperature as inverse proportion from 300 K to 600 K. Prskalo et al. [20] simulated the sputtering of SiC and Si_3N_4 based on MD. Their simulations agreed well with experiment of sputter yield on the complete low energy range. Amaya-Roncancio et al. [11] investigated the temperature effect on the hardness of Cr and CrN films, and a better mechanical response for films was found at low temperature. In this work, MD is employed to examine the structures and thermophysical properties of Cu/Au thin films.

2. Method and computational details

2.1. Preparation of Cu/Au thin films

The deposit system is composed of incident Au atoms deposit on Cu-substrate, as is shown in Fig. 1(a). The simulation box is

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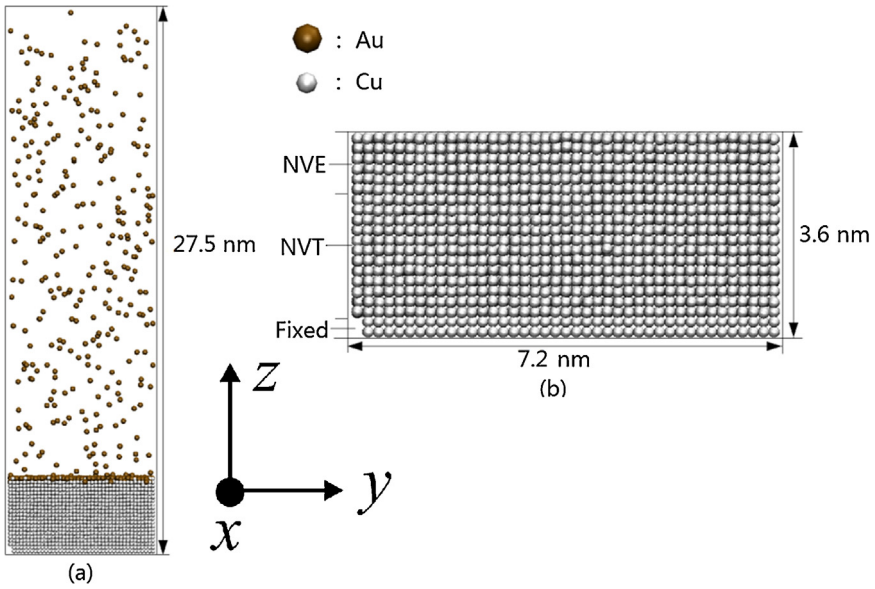

Fig. 1. Simulation model system of deposition. (a) System model. (b) Substrate model.

7.2 nm × 7.2 nm × 30 nm ($X \times Y \times Z$). The Au atoms are randomly generated in the region of 25–27.5 nm in Z-axis. The incident kinetic energy of Au atoms is 0.15 eV in Z-axis.

In Fig. 1(b), the substrate, 7.2 nm × 7.2 nm × 3.6 nm (20 × 20 × 10 unit cells in $X \times Y \times Z$), consists of 16,000 Cu atoms. After the substrate created, two layers of Cu atoms at the bottom of substrate are fixed, meanwhile the other Cu atoms of substrate equilibrate in NVT ensemble at 300 K for 1 ns. Then, the Cu atoms in top six layers of substrate are simulated in NVE ensemble for 1 ns, while the other atoms' interplaying remains unchanged. This model is updated from the nanochannel used for investigating the solid–liquid interface [15,21]. After that, Au atoms incident to the substrate in 1 ns with the deposition rate of 7.5×10^{24} atom/s cm^2 [22]. The Au particles are simulated in NVE ensemble. While the Cu atoms in three circumstances, i.e. NVE ensemble, NVT ensemble and fixed condition, interact with each other, as Fig. 1(b) presented.

Three modulation periods thin films are obtained based on the model of deposition, which are 1.8 nm Cu/3.6 nm Au, 2.7 nm Cu/2.7 nm Au and 3.6 nm Cu/1.8 nm Au. Also, the same modulation periods are used to generate ideal thin films without defect based on the lattice constant of Cu and Au. The thin films studied in this work are denoted as Deposit 1.8, Deposit 2.7, Deposit 3.6, Ideal 1.8, Ideal 2.7, and Ideal 3.6. For example, Deposit 1.8 represents the 1.8 nm Cu/3.6 nm Au thin film prepared by the deposition model.

2.2. Temperature gradient in the thin films

The six obtained thin films are annealed (heated to 1000 K and equilibrated for a short period, then cooled to 300 K) firstly. Then, the thin films are sliced into 6–7 layers (please see the supplementary material for details) in Z axis, as shown in Fig. 2. The top layer (Layer Heat) contacts with a heat source of 1000 K. The other layers are equilibrated in the NVE ensemble. The simulations run for 2,000,000 steps to generate the temperature gradient.

2.3. Forcefield and computational parameters

MD simulations are performed by using LAMMPS [23] (large-scale atomic/molecular massively parallel simulator). The EAM forcefield [24] is chosen as the interaction potential. Periodic boundary conditions are applied in X, Y coordinates. Two ideal walls are created perpendicular to the Z axis at bottom and up surfaces of the simulation box as the boundary. The time-step is set as 1 fs in the simulations. This time-step is tested for energy conservation. The Langevin method [25] is employed to conserve the temperature.

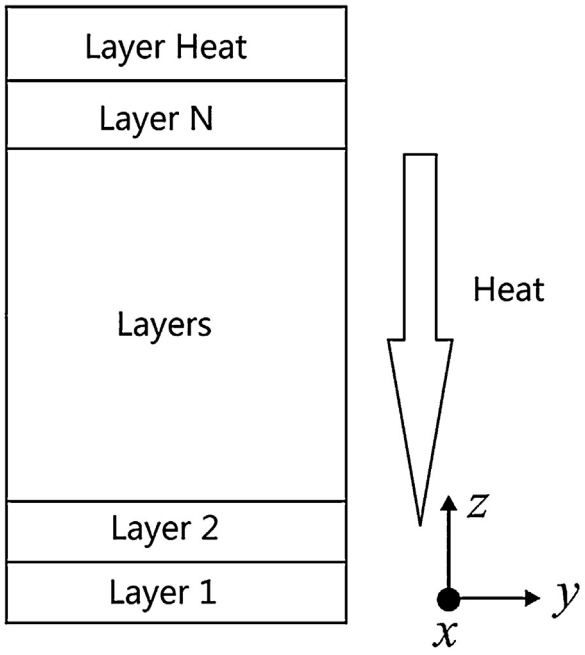

Fig. 2. Heat transportation in the thin films.

3. Results and discussion

3.1. Particle distribution of thin films after annealing

The particle distribution in thin films after annealing is presented in Fig. 3. The Cu–Au coherent lattice interfaces exist in all the thin films, even in the thin films modeled by the ideal lattice structures. The coherent lattice pattern can reduce the surface energy of interface formed by different atom types, and generate optimized structure. The coherent lattice interface of thin films obtained from deposition is thicker than that of ideal structures. Also, the Au atom distribution curves of thin films obtained via deposition, Fig. 3(a),