Applied Surface Science 276 (2013) 417–423

Contents lists available at SciVerse ScienceDirect

Applied Surface Science

journal homepage: www.elsevier.com/locate/apsusc

Comparison of Cu thin films deposited on Si substrates with different surfaces and temperatures

Jun Zhang*, Chong Liu, Jing Fan

State Key Laboratory of High-temperature Gas Dynamics, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, China

ARTICLE INFO

Article history:
Received 17 December 2012
Accepted 18 March 2013
Available online 25 March 2013

Keywords:
Copper thin film
Deposition and growth
Molecular dynamics
Crystalline structure and orientation

ABSTRACT

Deposition and growth of Cu thin films on Si(1 0 0), Si(1 1 0) and Si(1 1 1) substrates are studied using molecular dynamics method. The Cu/Si interface diffusion, surface roughness, crystalline structure and growth orientation of Cu thin films are investigated in detail. The effects of substrate surface and temperature are analyzed. Our simulation results show that the number of Cu atoms getting across the substrate surface for Si(1 1 1) substrate is the largest, and the number for Si(1 1 0) substrate is the smallest. This is caused by the difference of the linear atomic densities and planar atomic densities of Si crystal in different directions and planes. The growth of Cu thin films deposited on Si(1 0 0) substrate is ⟨1 0 0⟩ oriented at low temperature, and gradually changes to be ⟨1 1 1⟩ oriented as the increasing of substrate temperature. On the other side, the growth of Cu thin films deposited on Si(1 1 0) and Si(1 1 1) substrates is always ⟨1 1 1⟩ oriented. Increasing substrate temperature could effectively reduce surface roughness, increase the number of Cu atoms with face-centered cubic (fcc) structure, but meanwhile increase the Cu/Si interface diffusion. Under the same substrate temperature condition, the number of Cu atoms with fcc structure in thin films deposited on Si(1 1 0) substrate is larger than that deposited on Si(1 1 1) substrate.

1. Introduction

Due to the development of integrated circuits (IC), the demand of interconnection materials becomes higher. Interconnection materials serve as the streets and highways of IC, connecting elements of IC into a functioning whole and to the outside world. Historically, the most popular interconnection material is Al because of its low resistivity, ease of deposition and dry etching. However, as the line dimensions of interconnections continue to shrink to sub-micron range in the ultra-large scale integrated circuits (ULSIC), Al is no longer suitable due to its low electro migration resistance. In today's ULSIC, Cu has been used as interconnection material to replace Al as it offers lower resistivity and higher electron migration resistance. This replacement results in the research interests of epitaxial growth of Cu thin films on Si substrate. Many efforts have been devoted to depositing Cu atoms on Si substrate using various methods such as molecular beam epitaxy [1], electron beam evaporation [2,3] and magnetron sputtering [4]. These experiments reported that Cu(1 0 0) films could be grown on Si(1 0 0) substrate with a 45° rotation along ⟨1 0 0⟩ axis and Cu(1 1 1) films could be grown on Si(1 1 0) and Si(1 1 1) substrates.

Until now, most of studies of Cu thin films on Si substrate were performed by experimental methods. Due to the limitation of experiment conditions, these studies were limited to some specific cases, not systematical study. On the other hand, molecular dynamics (MD) method could be systematically performed to analyze the morphology of the deposited thin film in detail and to understand the growing mechanisms. Hwang [5] performed MD simulations for Cu cluster deposition on Si(1 0 0) substrate. Incident energy, substrate temperature, and cluster size were considered to discuss the critical conditions of epitaxy, mixing and sputtering modes. Their results showed that interface mixing occurred at the interface and the incident energy was the most important factor to affect the film growth modes, more specifically, quasi-epitaxy occurred at low incident energy, while the sputtering process could start when the incident energy was above 40 eV. Recently, we [6] have studied the properties of Cu thin films deposited and grown on Si(1 0 0) substrate. In our MD simulations, Cu atoms were deposited one by one, which corresponds to the experiment of electron beam physical vapor deposition [2,3], where the incident energies of Cu atoms below 1 eV. We showed that the growth of Cu thin films on Si substrate is three-dimensional island growth mode. Based on the common neighbor analysis of atoms, three crystalline structures in the deposited Cu films were indentified. More important, we found that the formed face-centered cubic (fcc) structure of Cu thin film is ⟨1 0 0⟩ oriented with a rotation by 45° along ⟨1 0 0⟩ axis when the substrate temperature is 300 K, while the fcc structure of Cu thin

* Corresponding author. Tel.: +86 10 82544025; fax: +86 10 62561284.
E-mail address: zhangjun04@imech.ac.cn (J. Zhang).

0169-4332/$ – see front matter © 2013 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.apsusc.2013.03.109

film becomes to be ⟨1 1 1⟩ oriented when the substrate temperature is 900 K.

In this paper, we extend our previous research of Cu thin film deposited on Si(1 0 0) substrate [6] to Si(1 1 0) and Si(1 1 1) substrates. Under different substrate surfaces conditions, we compared the Cu/Si interface diffusion, surface roughness, crystalline structure and orientation of Cu thin films. Meanwhile, the effect of substrate temperature is studied. Our objective is to find the optimal condition for the epitaxial growth of Cu thin film on Si substrate.

2. Potential and computational procedure

In this study, we used molecular dynamics with many-body effective potentials to model deposition of Cu on Si substrate. The embedded-atom method (EAM) potential and corresponding parameters developed by Adams et al. [7] are utilized to describe the atomic interaction of Cu atoms, and Tersoff potential [8,9] is used for the interaction of Si atoms. For the interaction between Si and Cu atoms, the effect of variable charge transfer also plays an important role. Recently, the extended Tersoff potential [10] and Charge optimized many-body (COMB) potential [11] have been developed by adding terms corresponding to the effects of charge transfer. However, the applications of these potentials to thin film deposition may be limited due to the fact that they require significantly larger computational efforts than traditional potentials. For example, the COMB potential costs 23 times more than EAM and 13 times more than traditional Tersoff potentials under same simulation conditions. For this reason, we employ Tersoff potential to describe the interaction between Si and Cu atoms. Charge transfer between Cu and Si is effectively taken into account through the parameter χ_{Cu-Si}, which is fitted to reproduce the experimental value of lattice constant of copper silicide ($Cu_{15}Si_4$). The details of Tersoff potential function and corresponding parameters are given in our earlier paper [6].

The three-dimensional model of the deposition process used in this work is similar to that described in the literature [6]. The Si substrate has the dimensions of 108.6 Å × 108.6 Å × 32.58 Å and consists of 19,200 atoms with diamond structure. For the comparison of different substrate surfaces, (1 0 0) plane, (1 1 0) plane and (1 1 1) plane of Si crystal are chosen as the deposition surface in simulations, respectively. Si atoms in substrate are classified into three types, namely fixed atoms, thermostat atoms, and Newtonian atoms. The fixed atoms comprise the bottom 4 layers of atoms, which are fixed on their lattice sites to prevent the moving of the substrate due to the hit of Cu atoms during deposition. The middle layers of atoms are defined as the thermostat atoms, which are used to control the substrate temperature. The Newtonian atoms comprise the top 8 layers of substrate atoms. The motions of thermostat atoms and Newtonian atoms are determined by the Newton's equations of motion, besides the velocities of thermostat atoms are rescaled every 10 time steps according to the prescribed substrate temperature. In our simulations, the equations of motion are solved using Verlet time-integration algorithm with a constant time step of $\Delta t = 1$ fs.

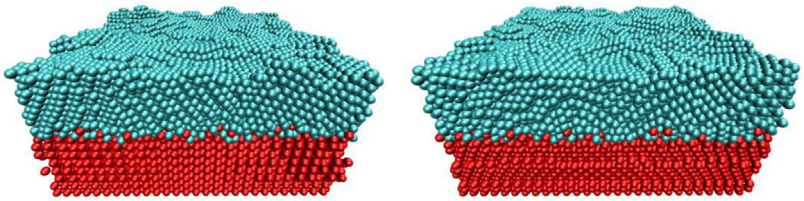
Deposition is performed by inserting one Cu atom every 400 calculating time steps, i.e., the deposition rate is 2.5 atoms/ps. The coordinates of deposited atoms are randomly generated within the insertion volume, which has the dimensions of 108.6 Å × 108.6 Å × 20 Å and is 54.3 Å height above the substrate surface. The initial velocities of deposited atoms are composed of macroscopic velocity and thermal velocity. In our simulations, the macroscopic velocities are chosen as 550 m/s vertically toward the substrate surface, while the thermal velocities are randomly selected from a Maxwellian distribution at the temperature of 220 K. These values are selected according to the general results in the experiments and simulations of electron beam physical vapor deposition [12]. Periodic boundary conditions are assumed in the x and y directions. Each simulation case proceeds with a certain substrate temperature until 22,000 Cu atoms are deposited on Si substrate. After deposition of the entire film, keep substrate temperature constant for 2000 ps to enable the deposited film to be relaxed, then linearly reduce the substrate temperature to 300 K with a cooling rate of 0.1 K/ps, and finally relax the whole system for another 2000 ps. All of our MD simulations are performed using the MD package-LAMMPS [13].

3. Results and discussions

In this section we present our simulation results. The growth mode of Cu thin film on Si substrate is three-dimensional island growth mode, which has been reported in detail in our earlier paper [6]. Here we focus on the Cu/Si interface diffusion, surface roughness, crystalline structure and growth orientation of Cu thin films deposited on different substrate surfaces. All of the analyses are based on the final state of thin film. Fig. 1 shows the morphology of the Cu thin films deposited on Si(1 1 0) and Si(1 1 1) substrates with $T = 300$ K.

3.1. Interface diffusion

It can be seen from Fig. 1 that interspecies mixing occurs at the interface between Cu film and Si substrate. The interface diffusion has an important effect on the epitaxial growth of Cu thin film. In addition, Cu/Si interfaces find application in optical detectors, solar cells, and chemical sensors [14]. Therefore, the chemical and physical properties of Cu/Si interface have been intensively studied. For example, Echigoya et al. [15] reported the formation of amorphous phase in Cu/Si(1 0 0) interface by reaction. Vaz et al. [16] performed a detailed investigation of the structural and morphological properties of Cu (1 0 0) layers grown epitaxially on Si(1 0 0) substrates, and they showed that interspecies mixing occurred at the Cu/Si interface, limited to less than 10 nm. To quantify the interface diffusion phenomenon, we count the number of Cu atoms getting across the original Si substrate surface under different substrate surface and temperature conditions. As shown in Fig. 2, the number of Cu atoms



(a) (b)

Fig. 1. Morphology of Cu thin films deposited on Si substrates with $T = 300$ K: (a) Si(1 1 0) substrate; (b) Si(1 1 1) substrate.

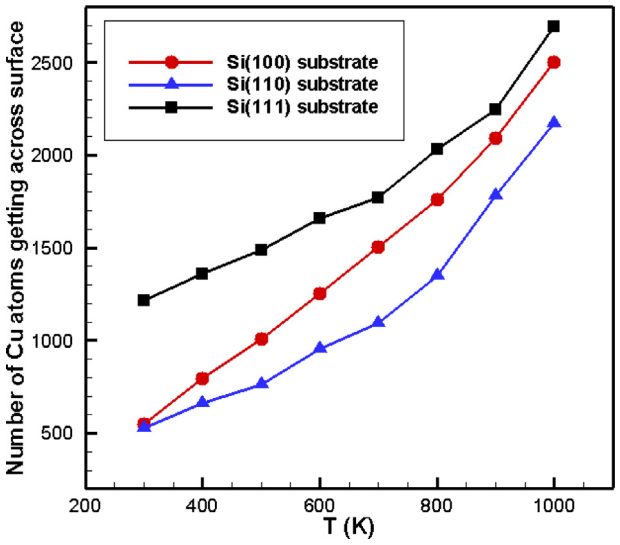


Fig. 2. Number of Cu atoms getting across the original substrate surface in Cu thin films deposited on Si(1 0 0), Si(1 1 0) and Si(1 1 1) substrates.

getting across the substrate surface increases as the increasing of substrate temperature. It is known that the diffusion coefficient of solid atoms could be expanded as

$$D = D_0 \exp\left(\frac{-E_d}{kT}\right), \quad (1)$$

where D_0 is pre-exponential factor, E_d is activation energy, k is Boltzmann constant, and T is temperature. According to Eq. (1), increasing substrate temperature would enhance the interface diffusion. Under the same substrate temperature condition, the numbers of Cu atoms getting across the substrate surface are different if the substrate surfaces for deposition are different. It can be seen from Fig. 2 that the number of Cu atoms getting across the substrate surface for Si(1 1 1) substrate is the largest, and the number for Si(1 1 0) substrate is the smallest. This phenomenon could be explained according to the linear atomic densities and planar atomic densities of Si crystal with diamond structure. Fig. 3 shows the atomic configurations of Si crystal in ⟨1 0 0⟩, ⟨1 1 0⟩ and ⟨1 1 1⟩ directions, and correspondingly the linear atomic densities are $1/a$, $\sqrt{2}/a$ and $2\sqrt{3}/3a$, respectively, where a is the lattice constant of Si crystal. Fig. 4 shows the atomic configurations of Si crystal in (1 0 0), (1 1 0) and (1 1 1) planes, and correspondingly the planar

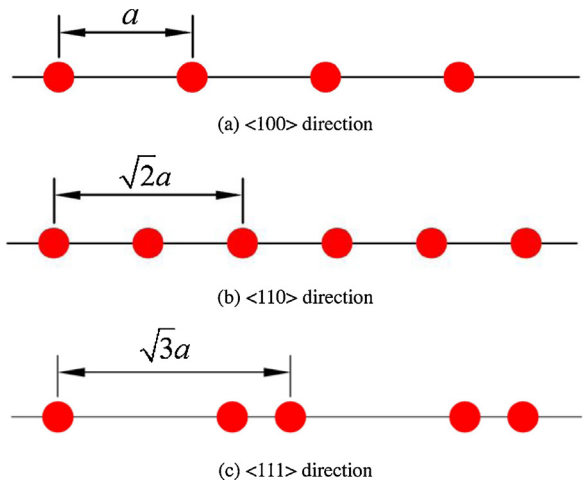


Fig. 3. Atomic configurations of Si crystal in different directions: (a) ⟨1 0 0⟩ direction; (b) ⟨1 1 0⟩ direction; (c) ⟨1 1 1⟩ direction.

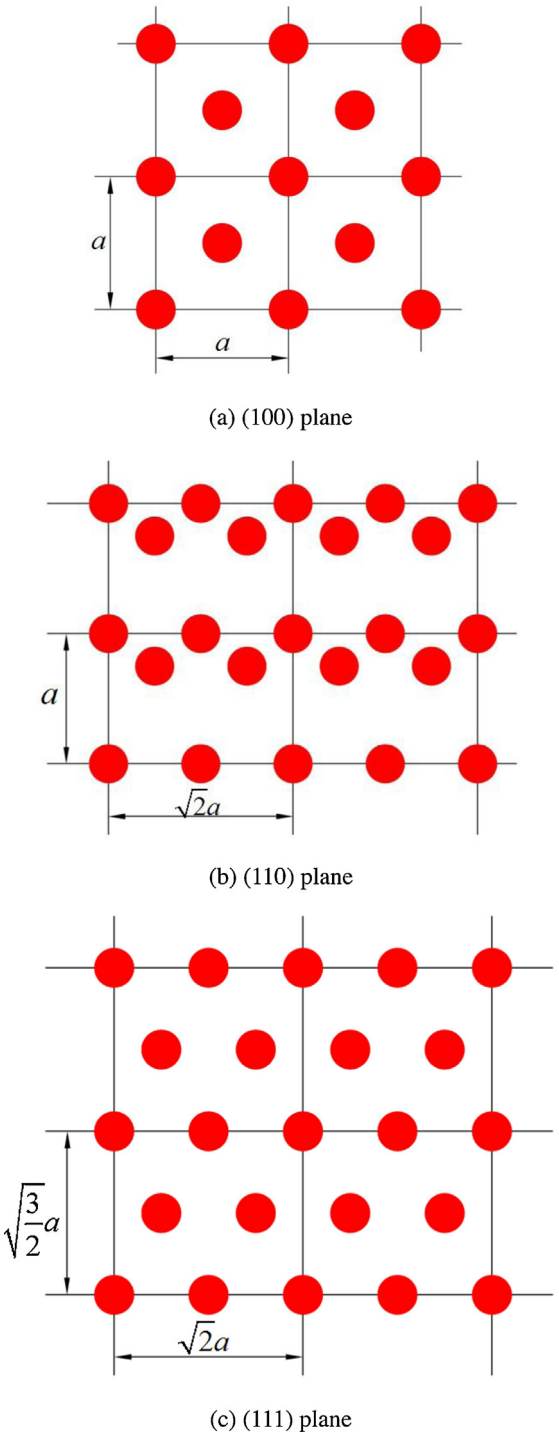


Fig. 4. Atomic configurations of Si crystal in different planes: (a) (1 0 0) plane; (b) (1 1 0) plane; (c) (1 1 1) plane.

atomic densities are $2/a^2$, $2\sqrt{2}/a^2$ and $4\sqrt{3}/3a^2$, respectively. Based on these results, we could conclude that the linear atomic density in ⟨1 1 0⟩ direction and the planar atomic density in (1 1 0) plane are the largest, and thus it is the most difficult for Cu atoms to get across the Si(1 1 0) substrate. On the other side, although the linear atomic density in ⟨1 1 1⟩ direction and the planar atomic density in (1 1 1) plane are larger than that in ⟨1 0 0⟩ direction and that in (1 0 0) plane, the number of Cu atoms getting across Si(1 1 1) substrate are larger than that for Si(1 0 0) substrate. This is because that the atomic distribution in ⟨1 1 1⟩ direction in non-uniform (see Fig. 3c), and the

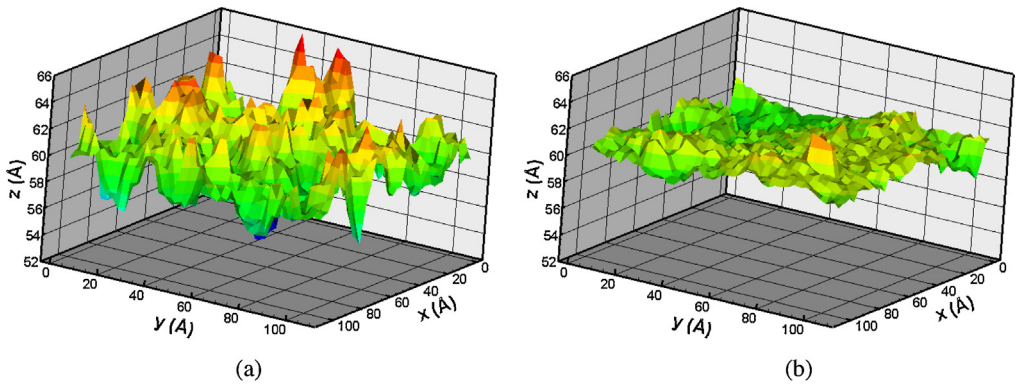


Fig. 5. Surface morphology of Cu thin films deposited on Si(1 1 0) substrate with different temperature: (a) $T = 300$ K; (b) $T = 900$ K.

largest distance of neighboring atoms is $3\sqrt{3}a/4$, which is larger than that in ⟨1 0 0⟩ direction (see Fig. 3a), a. Therefore, due to the larger vacancy in ⟨1 1 1⟩ direction, Si(1 1 1) substrate benefits the diffusion of Cu atoms comparing with Si(1 0 0) substrate. For the application of Cu thin films as interconnect material in integrated circuits, the Cu/Si interface diffusion is the bad side. In this context, Si(1 1 0) substrate is the optimal choice for the deposition of Cu thin films on Si substrate.

3.2. Surface roughness

Besides the interface between film and substrate, the quality of the deposited films is also closely related to the surface morphology. For example, Timoshevskii et al. [17] demonstrated by an ab initio study that atomic-scale surface roughness (1–3 atoms) on a perfect copper surface could lead to a substantial (30–40%) reduction in the electrical conductivity of thin Cu film. The physical origin of roughness-induced conductivity reduction may relate to the destruction of isotropic Fermi surface sheets. Therefore, reducing surface roughness is generally required for the fabrication of thin film. Fig. 5 shows the surface morphology of Cu thin films deposited on Si(1 1 0) substrate under different substrate temperature conditions. It is obvious that the surface of thin film obtained at $T = 900$ K is much smoother than that at $T = 300$ K. The surface roughness is quantitatively evaluated using the definition of root-mean-square roughness:

$$R_s = \sqrt{\frac{\sum_{i=1}^{n}(Z_i - \bar{Z})^2}{n}}, \quad (2)$$

where Z_i represents the height of the exposed atoms on the film surface, $\bar{Z}$ is the mean height of all the exposed atoms, and n is the total number of the exposed atoms. Fig. 6 shows the surface roughness obtained according to Eq. (2) under different substrate surface and temperature conditions. It is shown that the surface roughness decreases as the increasing of substrate temperature in the range of 300–900 K. This phenomenon is directly related to surface diffusion. Although surface diffusion coefficient is difficult to well-quantified, an empirical relationship similar to Eq. (1) is popularly used except that the specific values of pre-exponential factor and activation energy are somewhat different. In the range of 300–900 K, increasing temperature would enhance surface diffusion, and hence make the surface become smoother. However, when the substrate temperature exceeds 900 K, due to the strong interspecies mixing at the Cu/Si interface, the epitaxial growth of Cu thin film has been destroyed, and thus the surface roughness will be no longer decreasing linearly.

3.3. Crystalline structure and growth orientation

Crystalline structure and growth orientation are the most important properties for deposited thin films. Here the crystalline structures are analyzed using angular distribution functions as reported by Ackland and Jones [18]. The Ackland–Jones method (AJM) is based on the analysis of angular distribution function of perfect crystalline lattices as well as lattices with small distortions generated in simulations. With a heuristic algorithm it is decided which kind of local environment (structure) each atom belongs to. The power of AJM has been proven in analyzing structures based on MD simulation results and confocal microscopy data [18]. Recently, Pereira and da Silva [19] have successfully employed AJM to study the defects in Pd thin films on Au(1 0 0) substrate.

Using AJM analysis, we identified the Cu atoms in four different kinds of local environments: face-centered cubic (fcc), hexagonal close-packed (hcp), body-centered cubic (bcc) and amorphous structures. The atomic configurations in the cross section of the middle height of Cu thin films deposited on Si(1 0 0) substrate with $T = 300$ K and $T = 900$ K are shown in Fig. 7. Atoms are colored according to their local structures: green denotes fcc structure, brown denotes hcp structure, light blue denotes bcc structure, and dark blue denotes amorphous structure. It is obvious that the number of Cu atoms with fcc structure for $T = 900$ K is larger than that for $T = 300$ K. More interesting, Cu thin film with fcc structure is ⟨1 0 0⟩ oriented for $T = 300$ K, while it is ⟨1 1 1⟩ oriented for $T = 900$ K. This phenomenon has been reported in detail in our

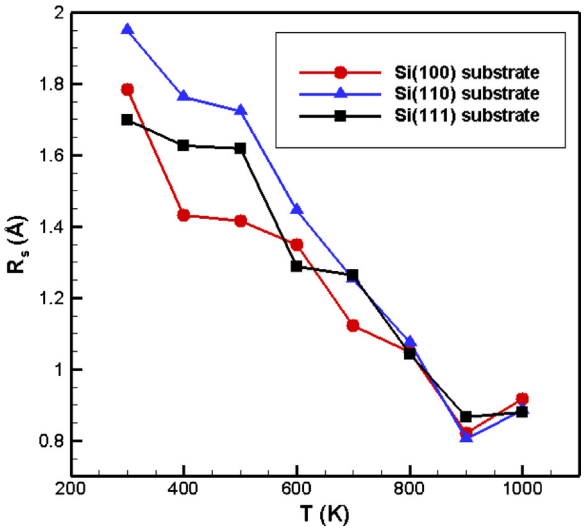


Fig. 6. Surface roughness of Cu thin films versus substrate temperature.

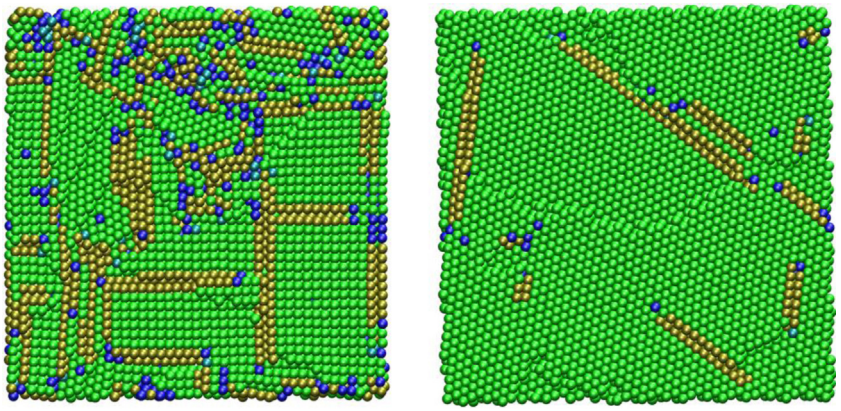


Fig. 7. Atomic configurations in the cross section of the middle height of Cu thin film deposited on Si(1 0 0) substrate: (a) $T = 300$ K; (b) $T = 900$ K. Atoms are colored according to their local structures: green denotes fcc structure, brown denotes hcp structure, light blue denotes bcc structure, and dark blue denotes amorphous structure. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

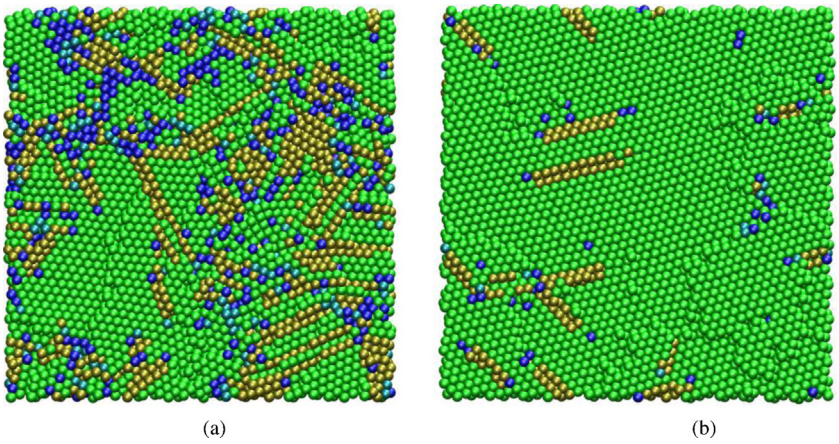


Fig. 8. Atomic configurations in the cross section of the middle height of Cu thin film deposited on Si(1 1 0) substrate: (a) $T = 300$ K; (b) $T = 900$ K. Atoms are colored in the same form as Fig. 7.

earlier paper [6]. The growth orientation could be identified by analyzing local atomic configurations of fcc structure along growth direction. The reason for the change from ⟨1 0 0⟩ orientation to ⟨1 1 1⟩ orientation is related to the surface free energy. It is known that for Cu crystal with fcc structure, the (1 0 0) planes have the highest surface free energy, while the closed-packed (1 1 1) planes have the lowest surface free energy. Therefore, deposited Cu films naturally prefer to grow with a ⟨1 1 1⟩ orientation to reduce surface free energy. However, when the substrate temperature is 300 K, there are not enough effective jumps for deposited atoms to move

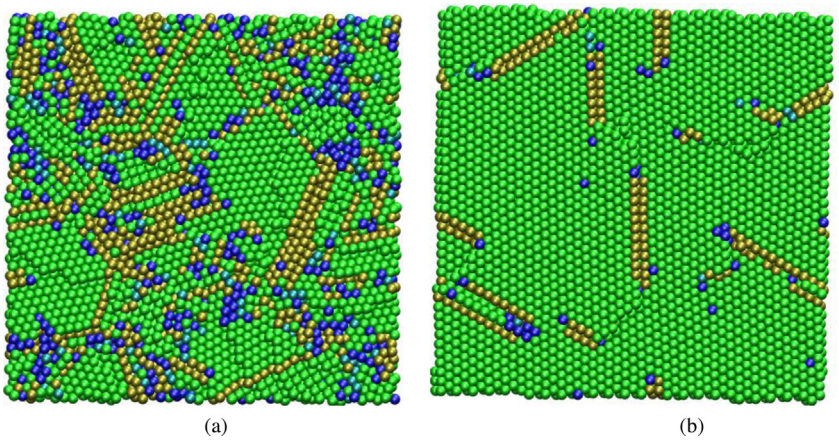


Fig. 9. Atomic configurations in the cross section of the middle height of Cu thin film deposited on Si(1 1 1) substrate: (a) $T = 300$ K; (b) $T = 900$ K. Atoms are colored in the same form as Fig. 7.

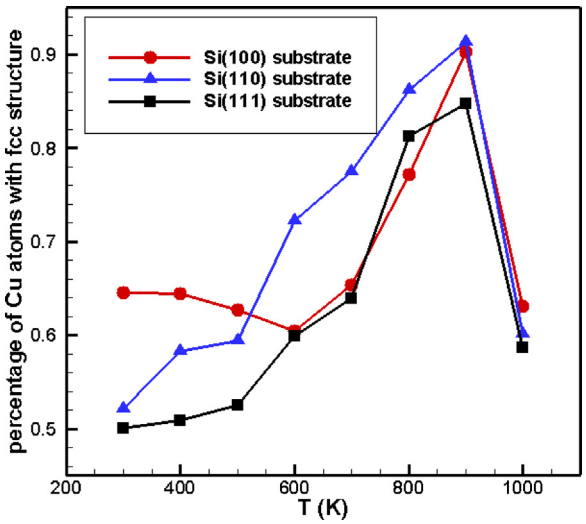


Fig. 10. Percentage of Cu atoms with fcc structure in thin films versus substrate temperature.

to their preferred locations, and most of them only vibrate in the neighborhood of their initial locations. In this way, the growth orientation for $T = 300$ K is mainly governed by the geometrical lattice match rule. When the substrate temperature gradually increases, the enough effective jumps for deposited atoms make them move to their preferred locations and form ⟨1 1 1⟩ oriented structure.

For the sake of comparison, we show the atomic configurations at the middle height of Cu thin film deposited on Si(1 1 0) and Si (1 1 1) substrate in Figs. 8 and 9, respectively. Atoms are also colored according to their local structures. It can be seen that all of Cu thin films with fcc structure are ⟨1 1 1⟩ oriented. This phenomenon is consisting of the experimental results reported by Jiang et al. using magnetron sputtering method [4]. Comparing the thin film deposited under different substrate temperature conditions, it is shown that the number of Cu atoms with fcc structure for $T = 900$ K is larger than that for $T = 300$ K.

To further quantify the effects of substrate surface and temperature on the structure of Cu thin film, we show the percentage of Cu atoms with fcc structure in thin films in Fig. 10. For the Cu thin films deposited on Si(1 1 0) and Si(1 1 1) substrates, the numbers of Cu atoms with fcc structures increase as the increasing of substrate temperature from 300 K to 900 K. When the substrate temperature exceeds 900 K, the epitaxial growth of Cu thin films is affected due to the strong interspecies mixing at the Cu/Si interface, and thus the number of Cu atoms with fcc structure will decrease. For the Cu thin films deposited on Si(1 0 0) substrate, the numbers of Cu atoms with fcc structures decrease as the increasing of substrate temperature from 300 K to 600 K. This is because that the growth of Cu thin film changes from ⟨1 0 0⟩ orientation to ⟨1 1 1⟩ orientation in the range of 300–600 K. When the substrate temperature exceeds 600 K, the numbers of Cu atoms with fcc structures increase as the increasing of substrate temperature up to 900 K. It is more interesting to note that under the same substrate temperature condition, the numbers of Cu atoms with fcc structures for Si(1 1 0) substrate is larger than that for Si(1 1 1) substrate. Accordingly, we could conclude that Si(1 1 0) substrate is preferable for the growth of Cu thin film with fcc structure. This conclusion is consistent with the experimental results reported by Jiang et al. using magnetron sputtering method [4]. As shown in their results related to XRD patterns and pole figures, the intensity of Cu(1 1 1) diffraction for Si(1 1 0) substrate is much stronger than that for Si(1 1 1) substrate at the same thickness.

4. Conclusions

We have systematically studied the deposition and epitaxial growth of Cu thin films on Si(1 0 0), Si(1 1 0) and Si(1 1 1) substrates using MD simulations. The Cu/Si interface diffusion, surface roughness, crystalline structure and growth orientation of Cu thin films are shown. The effects of substrate surface and temperature are analyzed in detail. Some important conclusions are as follows: for the Si(1 0 0) substrate, the growth of Cu thin films is ⟨1 0 0⟩ oriented at low temperature, and increasing substrate temperature could make the growth gradually change to be ⟨1 1 1⟩ oriented. Accordingly, as the increasing of temperature from 300 K to 900 K, the number of Cu atoms with fcc structure in thin films firstly decrease and then increase. When the substrate temperature approaches to 900 K, the number of Cu atoms with fcc structure arrives at its maximum. For the Si(1 1 0) and Si(1 1 1) substrates, the growth of Cu thin films is always ⟨1 1 1⟩ oriented. Under the same substrate temperature condition, the number of Cu atoms getting across the substrate surface for Si(1 1 0) is smaller than that for Si(1 1 1), and the number of Cu atoms with fcc structure for Si(1 1 0) is larger than that for Si(1 1 1). Therefore, Si(1 1 0) substrate is more favorable than Si(1 1 1) substrate for the epitaxial growth of Cu(1 1 1) thin films. Under the same substrate surface condition, increasing substrate temperature could reduce the surface roughness of thin films, increase the number of atoms with fcc structure, but meanwhile enhance the Cu/Si interface diffusion. Considering the comprehensive effects of substrate surface and temperature, we conclude that Si(1 1 0) substrate with 900 K is the optimal condition for the epitaxial growth of Cu thin films.

Acknowledgment

This work was supported by the National Natural Science Foundation of China (Grant Nos. 11002147 and 10921062).

References

[1] B.G. Demczyk, R. Naik, G. Auner, C. Kota, U. Rao, Growth of Cu films on hydrogen-terminated Si(1 0 0) and Si(1 1 1) surfaces, Journal of Applied Physics 75 (1994) 1956–1961.
[2] C.A. Chang, Formation of copper silicides from Cu(1 0 0)/Si(1 0 0) and Cu(1 1 1)/Si(1 1 1) structures, Journal of Applied Physics 67 (1990) 566–569.
[3] C.A. Chang, J.C. Liu, J. Angilello, Epitaxy of (1 0 0) Cu on (1 0 0) Si by evaporation near room temperatures: inplane epitaxial relation and channeling analysis, Applied Physics Letters 57 (1990) 2239–2240.
[4] H. Jiang, T.J. Klemmer, J.A. Barnard, E.A. Payzant, Epitaxial growth of Cu on Si by magnetron sputtering, Journal of Vacuum Science and Technology A: Vacuum, Surfaces, and Films 16 (1998) 3376–3383.
[5] S. Hwang, Molecular dynamic simulation for Cu cluster deposition on Si substrate, Computational Materials Science 56 (2012) 85–94.
[6] J. Zhang, C. Liu, Y.H. Shu, J. Fan, Growth and properties of Cu thin film deposited on Si(0 0 1) substrate: a molecular dynamics simulation study, Applied Surface Science 261 (2012) 690–696.
[7] J.B. Adams, S.M. Foiles, W.G. Wolfer, Self-diffusion and impurity diffusion of fcc metals using the 5-frequency model and the embedded atom method, Journal of Materials Research 4 (1989) 102–112.
[8] J. Tersoff, New empirical-approach for the structure and energy of covalent systems, Physical Review B 37 (1988) 6991–7000.
[9] J. Tersoff, Modeling solid-state chemistry – interatomic potentials for multicomponent systems, Physical Review B 39 (1989) 5566–5568.
[10] A. Yasukawa, Using an extended Tersoff interatomic potential to analyze the static–fatigue strength of SiO_2 under atmospheric influence, JSME International Journal – Series A: Solid Mechanics and Material Engineering 39 (1996) 313–320.
[11] T.-R. Shan, B.D. Devine, S.R. Phillpot, S.B. Sinnott, Molecular dynamics study of the adhesion of Cu/$SiO_{(2)}$ interfaces using a variable-charge interatomic potential, Physical Review B 83 (2011) 115327.
[12] J. Fan, I.D. Boyd, C. Shelton, Monte Carlo modeling of electron beam physical vapor deposition of yttrium, Journal of Vacuum Science and Technology A 18 (2000) 2937–2945.
[13] S. Plimpton, Fast parallel algorithms for short-range molecular-dynamics, Journal of Computational Physics 117 (1995) 1–19.
[14] H. Nienhaus, H.S. Bergh, B. Gergen, A. Majumdar, W.H. Weinberg, E.V. McFarland, Ultrathin Cu films on Si(1 1 1): Schottky barrier formation and sensor

applications, Journal of Vacuum Science and Technology A: Vacuum, Surfaces, and Films 17 (1999) 1683–1687.
[15] J. Echigoya, H. Enoki, T. Satoh, T. Waki, T. Ohmi, M. Otsuki, T. Shibata, Thin-film reaction and interface structure of Cu on Si, Applied Surface Science 56–8 (1992) 463–468.
[16] C.A.F. Vaz, S.J. Steinmuller, C. Moutafis, J.A.C. Bland, A.Y. Babkevich, Structural and morphological characterisation of hybrid Cu/Si(0 0 1) structures, Surface Science 601 (2007) 1377–1383.
[17] V. Timoshevskii, Y. Ke, H. Guo, D. Gall, The influence of surface roughness on electrical conductance of thin Cu films: an ab initio study, Journal of Applied Physics 103 (2008) 113705.
[18] G.J. Ackland, A.P. Jones, Applications of local crystal structure measures in experiment and simulation, Physical Review B 73 (2006) 054104.
[19] Z.S. Pereira, E.Z. da Silva, Study of defects in Pd thin films on Au(1 0 0) using molecular dynamics, Physical Review B 81 (2010) 195417.