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Growth and properties of Cu thin film deposited on Si(0 0 1) substrate: A molecular dynamics simulation study

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ABSTRACT

Molecular dynamics simulations are used to study the growth and properties of Cu thin film deposited on Si(0 0 1) substrate. In particular, growth mode, crystalline structure and orientation, and surface morphology of Cu thin film are investigated in detail. Our simulation results predict that the growth of Cu thin film on Si substrate is three-dimensional island growth mode. In the growth process, interspecies mixing occurs at the interface between Cu film and Si substrate, and the mixing length increases as the increasing of substrate temperature. Based on the common neighbor analysis of atoms, three crystalline structures in the deposited Cu films are indentified. More important, the formed face-centered cubic (fcc) structure of Cu thin film is (0 0 1) oriented with a rotation by 45° along ⟨0 0 1⟩ axis when the substrate temperature is 300 K, while the fcc structure of Cu thin film becomes to be (1 1 1) oriented when the substrate temperature is 900 K. The crystalline orientation of deposited film could be explained based on the surface free energy of different crystalline planes as well as the geometrical lattice match rule. In addition, surface roughness of Cu thin film decreases as the increasing of substrate temperature due to the enhancement of surface diffusion.

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1. Introduction

With the development of ultra-large scale integrated circuits (ULSIC), Cu has been gradually used as interconnection material to replace Al due to its low resistivity and high electron migration resistance. This replacement results in the research interests of epitaxial growth of Cu thin film 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]. Liu and Chen [5] reported the effect of substrate cleaning on the epitaxial growth of Cu thin films on Si(0 0 1) substrate. It was shown that Cu films grew preferentially along the ⟨1 1 1⟩ direction on atomically clean Si(0 0 1) surface and grew along the ⟨0 0 1⟩ direction on hydrogen terminated Si(0 0 1) surface. This report clarified some previous results obtained under different surface cleaning conditions.

In addition, the study of Cu/Si interfaces has been of crucial importance in micro-electronic devices due to their key role in the establishment of an ohmic contact, which is usually required for semiconductor electronic circuitry. Cu/Si interfaces also find application in optical detectors, solar cells, and chemical sensors [6]. Therefore, the chemical and physical properties of metal/semiconductor couples have been intensively studied. For example, Echigoya et al. [7] reported the formation of amorphous phase in Cu/(0 0 1)Si interface by reaction. Vaz et al. [8] performed a detailed investigation of the structural and morphological properties of Cu (0 0 1) layers grown epitaxially on Si (0 0 1) substrates. They showed that interdiffusion occurred at the Cu/Si interface, limited to less than 10 nm.

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. Recently, molecular dynamics (MD) method has been employed to investigate the deposition and growth process of thin films. Comparing with experimental research, MD simulations could be systematically performed to analyze the morphology of the deposited thin film in detail and to understand the growing mechanisms. Luedtke and Landman [9] performed MD simulations of metal on metal thin film growth. They showed that Au film deposited on Ni(0 0 1) substrate exhibited Stranski–Krastanov growth mode, and growth of Ni film on Au(0 0 1) substrate involved interspecies mixing and three-dimensional growth. Chu and Chen [10] employed MD simulations to study the morphology of growing Cu film on Cu substrate by the sputtering process, and they found that single crystal Cu film with good quality could be obtained by selecting reasonable combination of substrate temperature, deposition rate, incident energy, and incident angle. Although there are many MD simulations for

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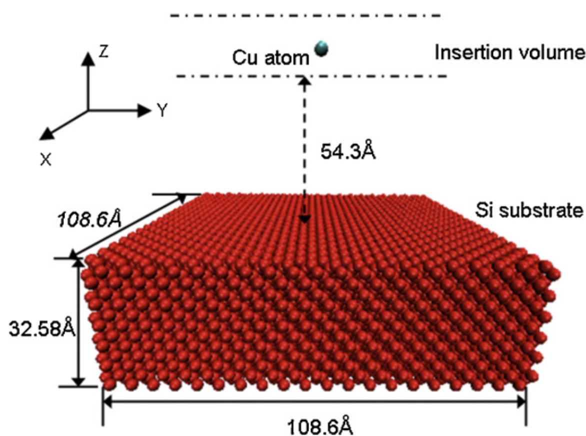

Fig. 1. Simulation model for deposition of Cu atom on Si substrate.

deposition of various thin films in the literature, such as Co thin film on Cu substrate [11], Al thin film on Ni substrate [12], Al thin film on Cu substrate [13], etc., simulations of deposition and growth of Cu thin film on Si substrate are very lacking. To the best of our knowledge, MD simulation of Cu thin film on Si substrate was only performed by Hwang et al. [14]. Their simulations of Cu cluster deposition corresponds to the experiments of Palasantzas et al. [15] and Majumdar et al. [16], where Cu atoms are sputtered in a magnetron device and then they combined in a flow of rare gas (Ar) to form clusters.

In this paper, we simulate the deposition of Cu atoms one by one using MD method. Our simulation corresponds to the experiment of electron beam physical vapor deposition [2,3]. We focus our research on the growth mode, crystalline structure and orientation, and surface morphology of Cu thin film deposited and grown on Si substrate. Effect of substrate temperature on the properties of thin film is investigated. Our objective is to provide useful information for the production of high-quality Cu thin film on Si substrate. This paper is organized as follows: Section 2 provides details of simulation model and potential function of Si–Cu system, and the potential parameters for the interaction between Si and Cu are fitted. Simulation results and discussions are shown in Section 3. Finally we present our conclusions in Section 4.

2. Simulation model and potential function

Fig. 1 shows the simulation model which consists of two parts, namely the Si substrate and the deposited Cu atom. The Si substrate has the dimensions of $20a \times 20a \times 6a$ (a = 5.43 Å, lattice constant of Si) and consists of 19,200 atoms with diamond structure. The (0 0 1) plane of substrate is perpendicular to the z-axis. There are three types of Si atoms in substrate, 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 12 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 Δt = 1 fs.

Deposition is performed by inserting one Cu atom every 400 calculating time steps, which means that 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 $20a \times 20a \times 6a$ and is $10a$ 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 [17]. Periodic boundary conditions are assumed in the x and y directions. Each simulation case proceeds until 22,000 Cu atoms are deposited on Si substrate and then a relaxation process of 1200 ps is conducted to enable the deposited thin film to be equilibrated. All of our MD simulations are performed using classic MD package-LAMMPS [18].

In MD simulations, potential function and corresponding parameters describing interactions between atoms are very crucial for accurately predict properties of materials. So far, many-body empirical potentials have been constructed for metallic and covalent systems. The embedded-atom method (EAM) potential proposed by Daw and Baskes [19] gives a realistic description behavior and properties of metallic bonding. For covalent bonding, the widely used potential for semiconductors was developed by taking into account the effects of coordination-number changes on the local short-range environment of the covalent bonds. In this work, the EAM potential and corresponding parameters developed by Adams et al. [20] are utilized to describe the atomic interaction of Cu atoms, and Tersoff potential [21,22] 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 [23] and Charge optimized many-body (COMB) potential [24] 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 similar to χ_{Ge-Si} in Ge–Si system [22] and χ_{O-Si} in O–Si system [25]. The details of Tersoff potential function and corresponding parameters are given in Appendix A.

3. Results and discussions

In this section we present our simulation results. The growth mode, crystalline structure and orientation, and surface morphology of Cu thin film are investigated in detail.

3.1. Growth mode

Fig. 2 shows the snapshots when 1250 and 22,000 Cu atoms (denoted in cyan) are deposited on the substrate (denoted in red) with the substrate temperature of 300 K, respectively. It is shown that the 1250 deposited Cu atoms (Fig. 2a) form small three-dimensional clusters with some substrate atoms still exposed, and the surface morphology of 22,000 atoms deposited film (Fig. 2b) is with roughness in some extent. To quantify the growth process of Cu film in detail, we divide the z direction into small intervals, each of which has the thickness of 0.2 Å. The distribution of Cu atoms in these intervals along z direction is shown in Fig. 3. For the sake of clarity, the original surface of Si substrate is shown as black dashed line. At the early stage (250 Cu atoms deposited), the Cu atoms

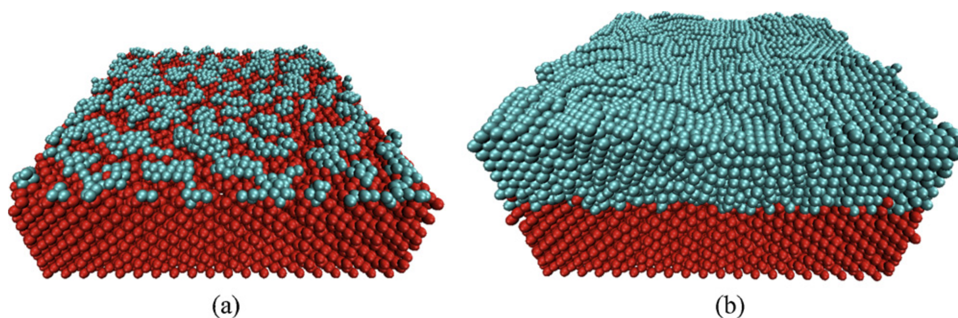

Fig. 2. Morphology of deposited Cu film in the growth process: (a) 1250 Cu atoms deposited; (b) 22,000 Cu atoms deposited. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article).

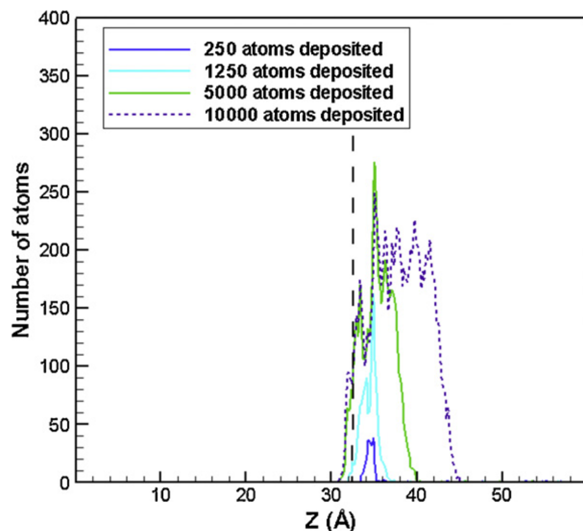

Fig. 3. Number of Cu atoms along the *z* direction in the growth process.

are randomly adsorbed on the surface of Si substrate. After 1250 Cu atoms are deposited, small islands are formed (Fig. 2a). From then on, film growth continues through the nucleation and coalescence of these islands, which can be explained by the Volmer and Weber growth mode [26], i.e., island growth mode. The substrate surface is completely covered by Cu atoms when 5000 Cu atoms are deposited. Simultaneously, due to the diffusion mechanism, some Cu atoms have gotten across the original surface of substrate as shown in Fig. 3. It can also be seen from Fig. 2b that interspecies mixing occurs at the interface between Cu film and Si substrate.

To further quantify the intermixing phenomenon, the distribution of number of Si atoms (red solid line) and Cu atoms (blue solid line) in intervals (0.2 Å thickness) along *z* direction at the final state is shown in Fig. 4. Also original surface of Si substrate is denoted in black dashed line. The bottom 4 layers of substrate atoms keep perfect layer structure because they are fixed on their lattice sites, while the other substrate atoms deviate slightly from their lattice sites due to motions. More important, some of the substrate atoms close to the surface diffuse into the deposited Cu film, and some of Cu atoms penetrate into the substrate. It is shown in Fig. 4 that the interspecies diffusion length increases from 6 Å with substrate temperature $T = 300$ K to 14 Å with $T = 900$ K. This mixing phenomenon between Cu film and Si substrate was also observed in experiments by Echigoya et al. [7] and Chen et al. [27] They further found that copper silicide was formed at the interface due to interfacial reaction.

3.2. Crystalline structure and orientation

Crystalline structure and orientation are the most important properties for deposited thin film. We employ the common neighbor analysis (CNA) method to analyze the local crystal structure of the deposited Cu film. The CNA method, firstly proposed by Honeycutt and Andersen [28], is a decomposition of the pair distribution function (PDF) according to the environment of the pairs and can provide direct interpretation of various features of PDF in terms of atomic structure. Faken and Jonsson [29] generalized such a

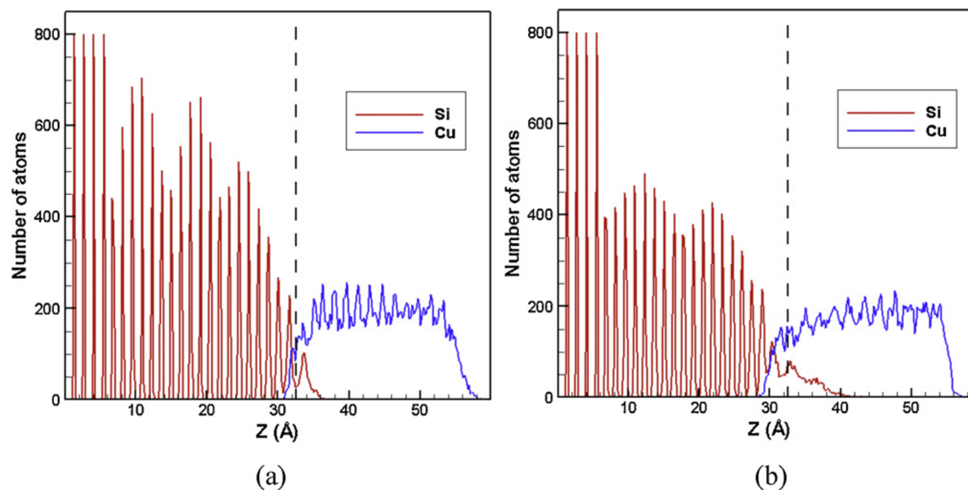

Fig. 4. Number of atoms along *z* direction after deposition of 20,000 Cu atoms and a relaxation process for 1200 ps. (a) substrate temperature is 300 K; (b) substrate temperature is 900 K.

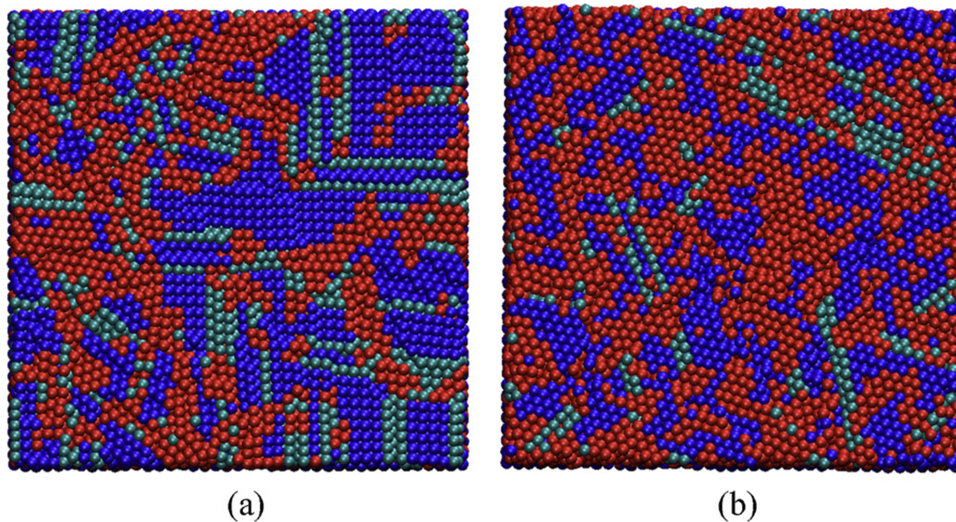

Fig. 5. Atomic configurations at the cross-section of $z = 50$ Å. (a) Substrate temperature is 300 K; (b) substrate temperature is 900 K.

method and systematically analyzed the local atomic structure of a molten Cu slab in combination with three-dimensional computer graphics. Using CNA analysis, we identified the Cu atoms in three different kinds of environment: face-centered cubic (fcc), hexagonal close-packed (hcp) and amorphous structure. The atomic configurations at the particular cross section ($z = 50$ Å) are shown in Fig. 5. Atoms are colored according to their CNA values: dark blue denotes fcc structure, cyan denotes hcp structure and read denotes amorphous structure.

To further understand the crystalline orientation of Cu thin film, we show the local atomic configurations of fcc structure along z direction in Fig. 6. Cu atoms are denoted in cyan, and Si atoms are denoted in red. Except that interspecies mixing occurs at the interface of Cu and Si atoms, clear crystalline orientation of Cu atoms along z direction could be identified. A very interesting phenomenon is that the fcc structure for $T = 300$ K is (0 0 1) oriented

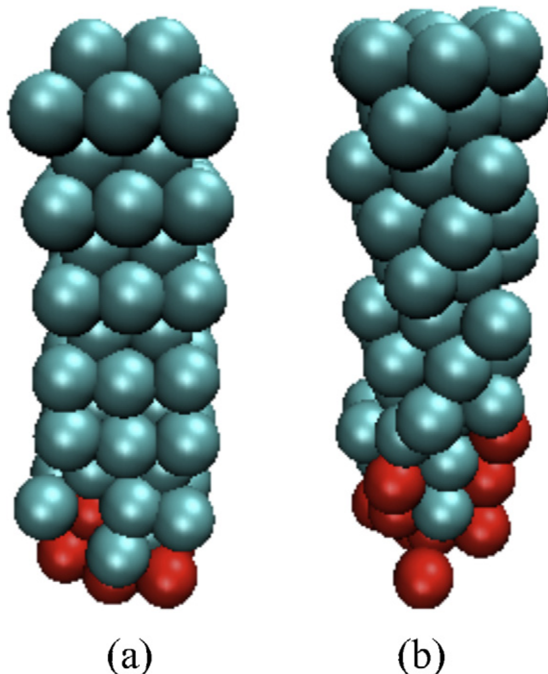

Fig. 6. Local atomic configurations of fcc structure along z direction. (a) Substrate temperature is 300 K; (b) substrate temperature is 900 K.

with a rotation by 45° along the ⟨0 0 1⟩ axis of substrate, while the fcc structure for $T = 900$ K is (1 1 1) oriented. It is known that for Cu crystal with fcc structure, the (0 0 1) planes have the highest surface free energy, while the closed-packed (1 1 1) planes have the lowest surface free energy. Therefore, deposited Cu film naturally prefer to grow with a (1 1 1) orientation to reduce surface free energy. However, in our MD simulations, the deposition rate is one atom per 0.4 ps, which means that one monolayer of Cu film is covered on substrate per 7.2×10^{-10} s. If the deposited atoms are desired to form (1 1 1) oriented structure, there is at least one effective jump for each Cu atom within 7.2×10^{-10} s. The mean time of one effective jump could be evaluated as follows:

$$\tau = \frac{1}{\nu_0} \exp\left(\frac{\varepsilon}{kT}\right) \quad (1)$$

where ν_0 is vibration frequency, ε is activation energy and k is Boltzmann constant. For metals with fcc structure typical values give as $\nu_0 \approx 10^{12}$ s^{-1} and $\varepsilon \approx 0.3$ eV. According to Eq. (1), the mean time of one effective jump for $T = 900$ K is about 4.8×10^{-11} s, which is one order smaller than the time within which one monolayer is formed. Consequently, there are enough effective jumps for deposited atoms to move to their preferred locations and form (1 1 1) oriented structure. On the other side, when the substrate temperature is 300 K, the mean time of one effective jump increases to 1.1×10^{-7} s, which is several orders larger than the time within which one monolayer is formed. This means that most of Cu atoms could not jump to their preferred locations and only vibrate in the neighborhood of their initial locations. For this reason, it is possible that (0 0 1) oriented Cu film grows on (0 0 1) Si substrate for $T = 300$ K. The rotation by 45° along ⟨0 0 1⟩ axis is governed by the geometrical lattice match rule. It is known that Cu has an fcc structure with a lattice constant of 3.615A, while Si has a diamond structure with a lattice constant of 5.43A. If the (0 0 1) oriented Cu film directly grows on the (0 0 1) plane of Si substrate, the lattice mismatch is 33%, which is much larger than the critical lattice parameter mismatch of 15% for epitaxial growth. However, if the (0 0 1) oriented Cu film rotates 45° along ⟨0 0 1⟩ axis, the lattice mismatch will decrease to 5.7%. In this way, it is applicable for (0 0 1) oriented Cu film epitaxially grows on the (0 0 1) plane of Si substrate.

These two kinds of crystalline orientation have also been observed in experiments of Liu and Chen [5] under room temperature condition. According to their experimental results, (1 1 1) oriented Cu thin film are grown on atomically clean Si(0 0 1)

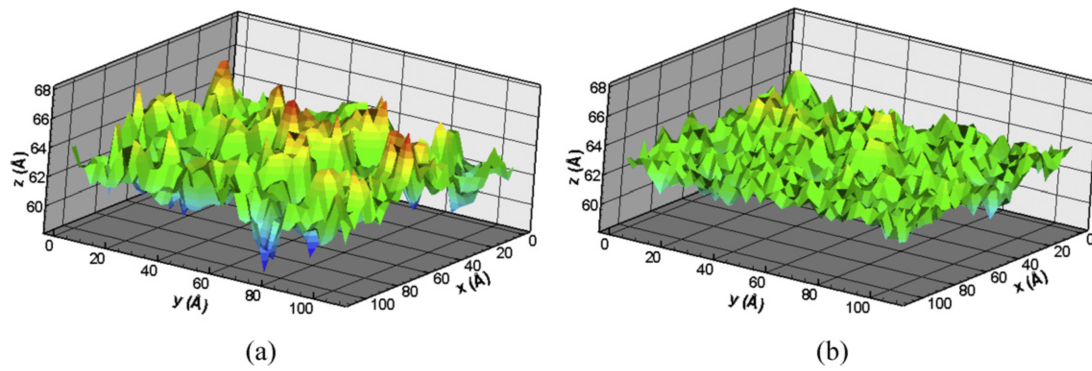

Fig. 7. Surface morphology of Cu thin film at the final state: (a) substrate temperature is 300 K; (b) substrate temperature is 900 K.

substrate. This is because the deposition rate in their experiments is several orders lower than that in our MD simulations, and hence the deposited Cu atoms have enough time to move to their preferred locations before one monolayer is formed. On the other hand, if the Si(0 0 1) surface is hydrogen terminated due to some particular treatment methods of surface cleaning, they found that the Cu thin film is (0 0 1) oriented with a rotation by 45° along the ⟨0 0 1⟩ axis of substrate, which is similar to the result in our MD simulations for $T = 300$ K.

3.3. Surface morphology

Besides crystalline structure and orientation, the quality of the deposited films is also closely related to the surface morphology. For example, Timoshevskii et al. [30] 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. Fig. 7 shows the surface morphology of deposited thin film at final state under different substrate temperature conditions. It is obvious that the surface at 900 K is much smoother than that at 300 K. The surface roughness is quantitatively evaluated using the definition of root-mean-square roughness:

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

where Z_i represents the height of the exposed atoms on the film surface, $\overline{Z}$ is the mean height of all the exposed atoms, and n is the total number of the exposed atoms. Fig. 8 shows the surface roughness under different substrate temperature conditions according to Eq. (2). It is shown that the surface roughness decreases as the increasing of temperature. This phenomenon is directly related to surface diffusion. Although surface diffusion coefficient is difficult to well-quantified, an empirical relationship for fcc metal surfaces is popularly used:

$$D_s = D_0 \exp\left(\frac{-E_d}{kT}\right), \tag{3}$$

where D_0 is the pre-exponential factor, and E_d is the activation energy. If D_0 and E_d keep invariant, D_s will increase as the increasing of T. In addition, we have showed in the previous subsection that the surface structure changes from (0 0 1) oriented to (1 1 1) oriented with the increasing of temperature. Usually, the activation energy for (1 1 1) plane is smaller than that for (0 0 1) plane. For these two reasons, surface diffusion coefficient increases as the increasing of temperature, and thus the surface of thin film becomes smoother as the increasing of temperature.

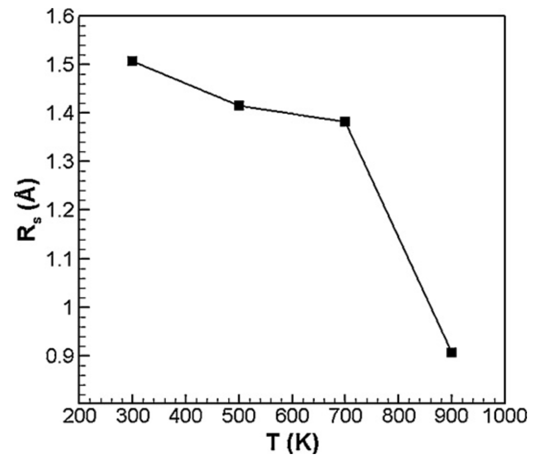

Fig. 8. Surface roughness versus substrate temperature.

4. Conclusions

The present work studied the deposition and growth of Cu thin film on Si(0 0 1) substrate using molecular dynamics method. Tersoff potential parameters for describing the interaction of Si and Cu atoms are fitted to reproduce the lattice structure of copper silicide. Growth mode, crystalline structure and orientation, and surface morphology of Cu thin film are investigated in detail. Our simulation results show that the growth of Cu thin film on Si substrate is three-dimensional island growth mode. At the interface between Cu film and Si substrate, interspecies mixing occurs due to diffusion mechanism. Two kinds of crystalline orientation are observed: when the substrate temperature is 300 K, the formed fcc structure of Cu thin film is (0 0 1) oriented with a rotation by 45° along ⟨0 0 1⟩ axis of substrate; when the substrate temperature is 900 K, the formed fcc structure of Cu thin film becomes to be (1 1 1) oriented. Surface roughness decreases as the increasing of substrate temperature. Knowledge of how the substrate temperature influences film property allows for better control over the production of Cu thin film on Si substrate.

Acknowledgments

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Appendix A. Tersoff potential and parameters for Si and Cu

The Tersoff potential computes of the energy of a system as

$$E = \frac{1}{2}\sum_{i}\sum_{j \neq i} V_{ij} \tag{4}$$

The interatomic potential between atom i and atom j has the following form:

$$V_{ij} = f_C(r_{ij})[f_R(r_{ij}) + b_{ij} f_A(r_{ij})], \tag{5}$$

where $f_R(r_{ij})$ indicates a repulsive pair potential and is two-body terms, while $f_A(r_{ij})$ represents an attractive pair potential and includes three-body interactions. Their forms are as follows:

$$f_R(r) = A\exp(-\lambda_1 r), \tag{6}$$

$$f_A(r) = -B\exp(-\lambda_2 r) \tag{7}$$

$f_C(r_{ij})$ in Eq. (5) is a cutoff function used to limit the range of the potential,

$$f_C(r) = \begin{cases} 1 & : r < R - D \\ \frac{1}{2} - \frac{1}{2}\sin\left(\frac{\pi}{2}\frac{r-R}{D}\right) & : R - D < r < R + D \\ 0 & : r > R + D \end{cases}, \tag{8}$$

where two cutoff parameters are represented as $R - D$ and $R + D$ that are selected to include only the first-neighbor shell.

The function b_{ij} in Eq. (5) represents a measure of bond order between atoms i and j and is assumed to be a monotonically decreasing function as

$$b_{ij} = \left(1 + \beta^n \varsigma_{ij}^n\right)^{-1/2n}, \tag{9}$$

with

$$\varsigma_{ij} = \sum_{k \neq i,j} f_C(r_{ik}) g(\theta_{ijk}), \tag{10}$$

$$g(\theta_{ijk}) = 1 + \frac{c^2}{d^2} - \frac{c^2}{d^2 + (h - \cos\theta_{ijk})^2} \tag{11}$$

where θ_{ijk} is the bond angle between bonds ij and ik. All of the values of Tersoff potential parameters including A, B, λ_1, λ_2, R, D, β, n, c and D for single component Cu and Si are listed in Table 1. For two component parameters, mixing rule is used as follows:

$$\lambda_1^{i,j} = \frac{1}{2}\left(\lambda_1^i + \lambda_1^j\right), \tag{12}$$

$$\lambda_2^{i,j} = \frac{1}{2}(\lambda_2^i + \lambda_2^j), \tag{13}$$

$$A^{i,j} = (A^i A^j)^{1/2}, \tag{14}$$

Table 1
Parameter values for Tersoff potential.

	Si	Cu
A(eV)	1830.8	803.12
B(eV)	471.18	43.25
λ(Å^{-1})	2.4799	2.83
μ(Å^{-1})	1.7322	1.412
β	1.1000E-6	0
n	0.78734	1
c	1.0039E5	0
d	16.217	1
h	−0.59825	0
R(Å)	2.85	3.075
D(Å)	0.15	0.255
	χ_{Cu-Si} = 1.02239	

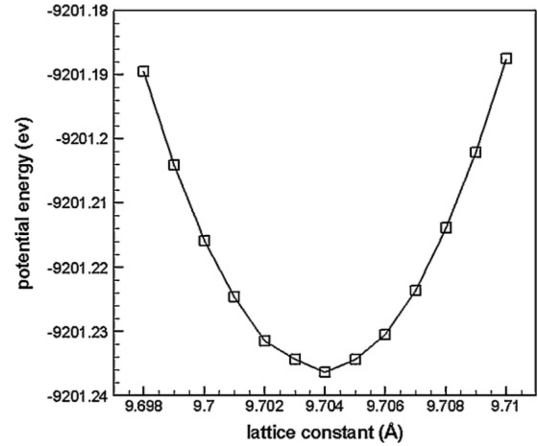

Fig. 9. Potential energy of $Cu_{15}Si_4$ crystal versus lattice constant for χ_{Cu-Si} = 1.02239.

$$B^{i,j} = \chi_{ij}(B^i B^j)^{1/2}, \tag{15}$$

$$Q^{i,j} = (Q^i Q^j)^{1/2}, \tag{16}$$

$$S^{i,j} = (S^i S^j)^{1/2}, \tag{17}$$

where Q and S are related to R and D as this form: $Q = R - D$ and $S = R + D$. The only new parameter in Eqs. (12)–(17) is χ_{ij}, which is used for the weakening or strengthening of heteropolar bonds. Charge transfer between Cu and Si is effectively taken into account through the parameter χ_{Cu-Si} in our model. The adjustable parameter χ_{Cu-Si} is fitted to reproduce experimental value of lattice constant of copper silicide ($Cu_{15}Si_4$). In our MD simulation for fitting χ_{Cu-Si}, a $3 \times 3 \times 3$ cubic cell is constructed according to the structure of $Cu_{15}Si_4$, and the total number of atoms is 2052. For any value of χ_{Cu-Si}, we obtain the potential energy of system under various lattice constant conditions. Fig. 9 shows the potential energy of system versus lattice constant for χ_{Cu-Si} = 1.02239. According to the minimum potential principle, the lattice constant is determined as 9.704 Å, which is in agreement with the experimental value for $Cu_{15}Si_4$. In this way, the value of χ_{Cu-Si} is determined as 1.02239, which is used in our simulation of deposition and growth of Cu thin film.

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