고전 분자동역학 방법을 사용한 실리콘 표면위의 이온화된 Al의 물리기상증착에 관한 연구

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Classical Molecular Dynamics Study of Al Ionized Physical Vapor Deposition on Silicon Surface

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Abstract

We calculated Al-Absorption, Al-reflection, and Si-etching probabilities as a function of incident angle and energy using classical molecular dynamics (MD) simulation. Variations of the cases of Al-absorption rate and Al-reflection rate are less than that of Si-etching rate. In contrast with general prediction, our simulation results showed that channeling of the <110> direction occurred the most in the case of incident angle between 30degree and 40degree. We investigated that channeling of the <110> directions quite affect Al-absorption rate in silicon. Since Si-etching rate is high and Al-absorption rate by <110> channeling is high, we found that Al ionized physical vapor deposition (PVD) on Si(001) has a different characteristics with Al ionized PVD on Al(111).

I. Introduction

Metal-semiconductor interface is important in electronic devices as Shottky barrier. The study of metal/semiconductor interfaces has received considerable attention because of their wide-range applications in electronic devices and composite materials.[1-3] Metal film growth during physical vapor metallization of contact via typical of semiconductor devices technology has been studied. The investigation of group-III metals on Si surface has been one of the typical studies in surface science for many years. Of the group-III metals, Al is a particularly important material for device applications. As electronic device dimensions scale down nanometer size, the study of nanostructure of metal-semiconductor interface has been necessary. For atomic-scale study of metal deposition, molecular dynamics (MD) method and kinetic Monte Carlo (KMC) method have been applied.[4,-14] Previous studies of metal deposition were about the cases of Al deposition on Al(111)[4,5], Cu and Au deposition on Cu(001)[6], Cu cluster deposition[11,12], Ag deposition[13], and the energetic deposition of fcc metals[14]. However, the atomistic simulations of metal deposition on semiconductors have not been studied. In this paper, we investigate Al physical vapor deposition on the Si(001) surface. The reaction probabilities were calculated in classical molecular dynamics simulations using empirical interatomic potentials. In particular we determined, as a function of the energy and off-normal angle of incident Al atoms, the probabilities of three processes: Al-absorption, Al-reflection, and Si-etching.

This paper is organized as follows. The description of the methods is presented in Sec. II, where we give the interatomic potential model and condition of molecular dynamics. The results are presented in Sec. III. Finally, a summary is given in Sec. IV.

II. Methods

A. The potentials

In this paper, we have employed two widely used potential formalisms proposed by Stillinger-Weber[15] and by Ito,Kho, and Das Sarma[16,17,18]. Below, we briefly summarize these formalisms and discuss their implementation in the present calculations. The SW potential formalism is

$$V_i = \sum_{i \neq j} v_2(i,j) + \sum_{i<j<k} v_3(i,j,k)$$

where V_i is potential energy of atom i and v_2 and v_3 represent two-body and three-body potential function, respectively. The complete descriptions of the SW potential are given in Ref. 15. For the simulation involving Al, we have used the Ito-Khor-Das Sarma potential given by the formalism

$$V_{ij} = A\exp[-\beta(r_{ij}-R_i)^{\gamma}]\left[e^{-\theta r_{ij}} - \frac{B_0}{Z_i^{\alpha}} e^{-\lambda r_{ij}} \{1 + \sum_{k,i,j(k\neq i,j)} [\cos\eta(\theta_{ijk}-\theta_i)-1]\}\right]$$

where θ_i is the equilibrium angle between nearest-neighbor bonds for a regular structure with coordination number $Z_i = \sum_j \exp[-\beta(r_{ij}-R_i)^{\gamma}]$, θ_{ijk} is the angle between bonds ij and ik, η is a parameter to fit the bond-bending force constant, and the summation is only over nearest-neighbor atoms whose bond ik is equal to the nearest bonds of ij. R_i is the minumum interatomic distance of these neighbors. The quantity $\exp[-\beta(r_{ij}-R_i)^{\gamma}]$ is the counterpart of the Tersoff's bare bonding potential. The parameter β and γ can be fitted to given the correct effective coordination numbers. The Al-Si parameters are taken from Ref. 1. The parameter eta is set to zero for the Al-Si interactions because there is no definite bond angel between Al-Si.

B. Conditions for Calculations

The total atom number in MD cell using the silicon substrate is 1,000. We assumed that the substrate be (100) silicon and the simulated temperature be 300 K. Periodic boundary conditions were applied to the sides. Positions and velocities of every atom in the MD cell were calculated following each time step by integrating the Newtonian equations of motion using the Velet algorithm. The time step in the integration is set to 0.1 fs. All atomic coordinates are allowed to evolve dynamically, except for those of the bottom layers of the MD cell.

We start our simulations with the incident Al atom placed outside the interaction range of the surface. Its initial kinetic energy is in the range of 20 eV to 120 eV, and its starting angle off the surface normal in the angle 0° to 60°, which corresponds to typical ionized physical vapor deposition condition. The trajectories of the incident atom, and of any other atom which may be etched away from the surface upon impact, are then monitored until kinetic energies of all Si atoms have below 5 eV after either incident Al atom is stopped or is reflected. When the kinetic energy of the incident Al atom has a below 5 eV and the force on the incident Al atom is a below 5 eV/Å (= 8.0×10^{-9} N), then that is stopped. If outcomming atoms (in the case of reflection or etching) have traveled a distance of 4 Å away from the surface, those atoms also are stopped. Analyzing 200 trajectories per incident energy and angle, we collected a statistically significant date of well-defined adsorption, reflection, and etching events. The relative probability of the corresponding process is calculated as the ratio of the number of events of each kind to the total incident number equal to 200. The typical statistical error in the reaction probabilities thus determined is below 5%.

III. Results and Discussions

Analyzing 200 trajectories per incident energy and angle, we calculated a statistically significant date of well-defined Al-Absorption, Al-reflection, and Si-etching probabilities as a function of incident angle and energy as in Fig. 1. In this work, Al-absorption probability includes Al-adsorption on Si(001) and Al in silicon. As incident angle increases, Al-absorption rate decreases, Al-reflection rate increases, and Si-etching rate rapidly increases.

In the cases of 60° of 100 eV and 120 eV, Si-etching rate is greater than Al-absorption rate, and these cases can be considered to be etching processes. Figure 2 shows the Si-etching rate as a function of incident energy. Si-etching rate is linearly proportional to incident energy but nonlinearly proportional to incident angle and this is consistent in result of physical etching process. In Fig. 1, we can see that variations of the cases of Al-absorption rate and Al-reflection rate are less than that of Si-etching rate. Si-etching rate calculated in this work is greater than Al-etching rate calculated in previous works[4,5] that investigated Al physical vapor deposition on the Al(111) surface. Al(111) surface is the one of the lowest formation energy. However, Si(001) surface has dangling-bonded silicon atom and Si-dimer, which interact with energetic Al atoms and they are etched by physical interaction such as sputtering. Therefore, Si-etch in Si(001) surface were occurred by energetic Al atoms.

Figure 3(a) and (b) show the number of Al atom more than 4 Å and 8 Å away from the inside of Si(001) surface as a function of incident energy and angle, respectively. As incident energy increases, effect of implantation increases and stopping depth of incident Al atoms increase. In Fig. 3(a), in all cases of incident energy, peak value of the number of Al atom more than 4 Å away from the inside of Si(001) surface is obtained in the case of 30°. However, in Fig. 3(b), peak value of the number of Al atom more than 8 Å away from the inside of Si(001) surface is obtained in the case of between 30° and 40°. For the case of Fig. 3(b), Fig. 4 shows configuration of Al atoms and Si lattices more than 8 Å away from the inside of Si(001) surface in the case of incident energy 80 eV and incident angle 40°. We can see that most of the Al atom more than 8 Å away from the inside of Si(001) surface went to the <110> directions occurring atom channeling. We can easily estimate that the <110> channeling may occur the most in the case of incident angle 45°. However, in contrast with this estimation, our simulation results show that channeling of the <110>

direction occurs the most in the case of incident angle between 30° and 40°. Figure 1 showed Si-etching rate increases while Al-absorption rate decreases above incident angle 40°. The fact that Si-etching rate increases means that the energy loss of incident Al atom increases and the fact that Al-reflection rate increases mean that the probability of channeling decreases. Therefore, channeling of the <110> direction occurs the most in the case of incident angle between 30° and 40°.

IV. Summary

We calculated Al-Absorption, Al-reflection, and Si-etching probabilities as a function of incident angle and energy. As incident angle increases, Al-absorption rate decreases, Al-reflection rate increases, and Si-etching rate rapidly increases. We could see that variations of the cases of Al-absorption rate and Al-reflection rate are less than that of Si-etching rate. Si-etching rate calculated in this work is greater than Al-etching rate calculated in previous works that investigated Al physical vapor deposition on the Al(111) surface. Since Si(001) surface has dangling-bonded silicon atom and Si-dimer, surface Si atoms interact with energetic Al atoms and are etched by physical interaction such as sputtering. In contrast with general prediction, our simulation results showed that channeling of the <110> direction occurred the most in the case of incident angle between 30° and 40°. Si-etching rate increases while Al-absorption rate decreases at above incident angle 40°. We could expect increase of the energy loss of incident Al atom from the fact that Si-etching rate increases and decrease of the probability of channeling from the fact that Al-reflection rate increases. Since Si-etching rate is high and Al-absorption rate by <110> channeling is high, Al ionized physical vapor depositeion (PVD) on Si(001) has a different characteristics with Al ionized PVD on Al(111).

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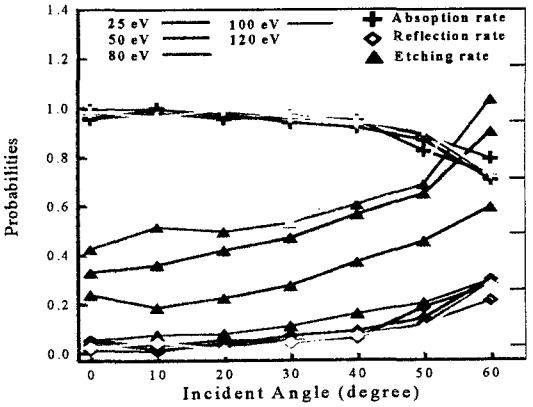


Figure 1. Al-Absorption, Al-reflection, and Si-etching probabilities impinging on Si(001) surface as a function of incident angle and energy.

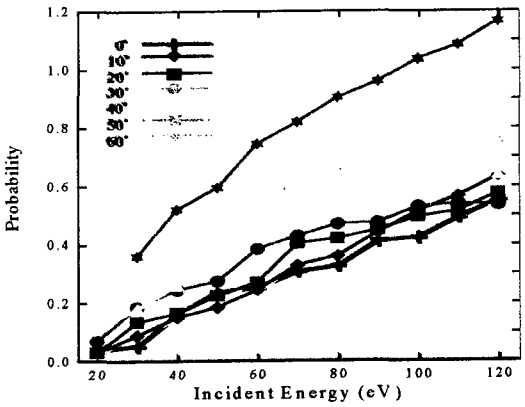
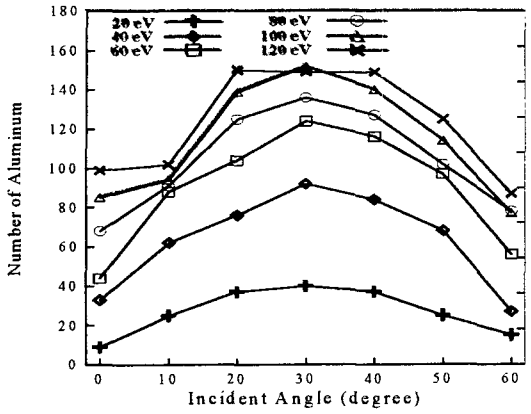
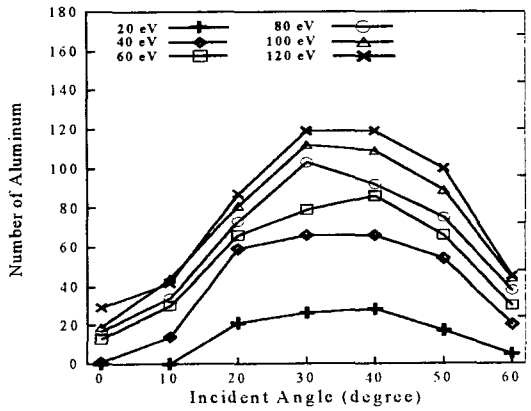


Figure 2. Si-etching rate for Al atoms impinging on Si(001) surface as a function of incident energy and angle.

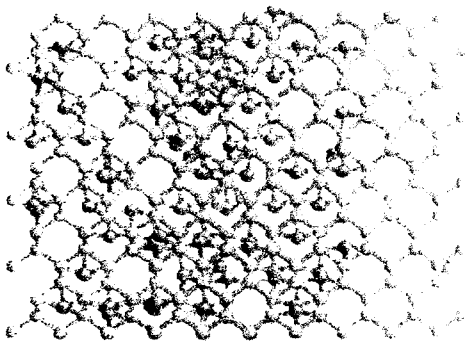


(a)

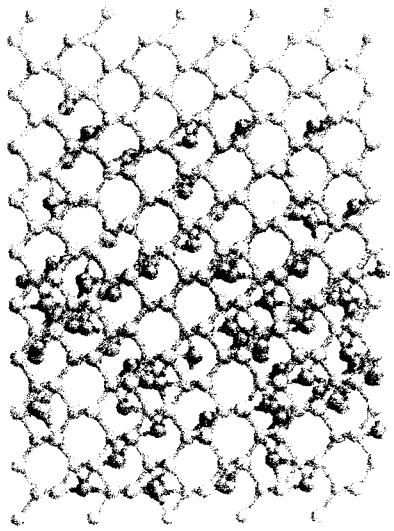


(b)

Figure 3. The number of Al atom in silicon.
(a) and (b) show the number of Al atom more than 4 Å and 8 Å away from inside of Si(001) surface as a function of incident energy and angle, respectively.



(a)



(b)

Figure 4. Configuration of Al atoms and Si lattices more than 8 Å away from the inside of Si(001) surface in the case of incident energy 80 eV and incident angle 40° . (a) [011] view. (b) [101] view.