第 21 卷第 11 期　　半 导 体 学 报　　Vol. 21, No. 11
2000 年 11 月　　CHINESE JOURNAL OF SEMICONDUCTORS　　Nov., 2000

Simulation of Nano Si and Al Wires Growth on Si(100) Surface*

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Abstract: Growth of nano Si and Al wires on the Si(100) surfaces is investigated by computer simulation, including the anisotropic diffusion and the anisotropic sticking. The diffusion rates along and across the substrate dimer rows are different, so are the sticking probabilities of an adatom, at the end sites of existing islands or the side sites. Both one-dimensional wires of Si and Al are perpendicular to the dimer rows of the substrate, though the diffusion of Si adatoms is contrary to that of Al adatoms, i.e. Si adatoms diffuse faster along the dimer rows while Al adatoms faster across the dimer rows. The simulation results also show that the shape anisotropy of islands is due to the sticking anisotropy rather than the diffusion anisotropy, which is in agreement with the experiments.

Key words: nano wires; anisotropy; simulation; Si(100) surface
PACC: 6855; 6835
CLC number: TN304　**Document code**: A　**Article ID**: 0253-4177(2000)11-1116-06

1 Introduction

Because of the importance in microelectronics and their unique properties, the nano silicon wires or other nano metal wires grown on Si(100) surface have been extensively investigated and it is now a field of very active research[1—4]. The Si(100) surface is the basis for most of the nano-fabrication methods and consequently has become the object of many experimental and theoretical studies. The growth of Si on Si(100) has been used as a model for a better understanding of the atomistic mechanisms of film growth[1,2]. Previous

* Project Supported by National Natural Science Foundation of China Under Grant No. 49672095, Natural Science Foundation of Zhejiang Province Under Grant No. 198034, and by Foundation of Engineering Science Center of Zhejiang University of Technology.

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Received 28 January 2000, revised manuscript received 1 May 2000

Scanning Tunneling Microscopy (STM) experiments[5,6] and the theoretical calculation[7,8] indicate that the Si(100) surface exhibits highly anisotropic diffusion. Much attention has been focused on the possible pathway to the nucleation of a Si ad-dimer under a wide range of growth conditions for the homoepitaxy on Si(100)[9—13]. Despite the intrinsic ability of STM to observe the morphology of the island formed, little has been known about its evolution from a single ad-dimer to the large structures, and the anisotropic growth on the Si (100) reconstruction surface. On the other hand, simulation is used more and more widely in the study of diffusion and the nucleation of atoms (including dimers), formation of islands and thin-film growth. The precisely defined growth conditions, low coverages and slow deposition rates in such studies make it possible to simulate the evolution of one-dimensional (1D) wires and two-dimensional (2D) thin-film's growth, and explore ways to tailor the film morphology and growth mechanism at an atomic level. In this paper, the growth of nano Si and Al wires on Si(100) surfaces is investigated by computer simulation with the purpose of studying the atomic processing from adatom adsorption and diffusion to the growth of 1D nano islands.

2 Simulation Model

The simulation model adoped is described as follows: adatoms are deposited onto a 360×360 Si(100) surface one by one with a deposition flux F (monolayers/sec), and allowed to diffuse along or across the substrate dimer rows with different diffusion rate. The surface diffusion rate is given as an Arrhenius form:

$$\nu = \nu_0 \exp(-E_m/kT)$$

where ν_0 is the vibrational frequency of a surface atom ($\sim 10^{13} s^{-1}$, and we assume it independent of the diffusion directions), E_m is the migration energy of a surface atom, T is the surface temperature and k is Boltzmann constant. It is known that the Si(100) surface is reconstructed to form the parallel rows of surface dimers. The migration barriers of the adatom along or across the dimer rows are different, i.e., the diffusion of adatoms on Si (100) surface is anisotropy. When a diffusing atom catches another mobile atom, the two atoms will stick together and become a dimer. The dimers have two orientations: parallel or perpendicular to the substrate dimer rows, as shown in Fig. 1. The perpendicular dimers formed on the Si(100) surface are energetically more stable than the parallel ones[1]. Roughly, should we set a probability P to form the perpendicular dimer ($P > 0.5$), there is a probability $1-P$ to form the parallel one. The process of dimer diffusion (including rotation) is not covered. These dimers then serve as the center for the growth of larger islands, as more adatoms will meet them. The diffusion steps of adatoms on the substrate are not limited due to the very long residence time of the atoms on the surface and the evaporation of atoms from the substrate is neglected as well. The effect of dissociation of nucleus is also negligible. Because of the reconstructed silicon surface absorbing atoms (or dimers), the sticking probabilities for a mobile atom are different at end sites

and side sites of the existing islands, i. e., both the diffusion and the stick during the growth of Si and Al on Si(100) surface are anisotropy[14]. The periodic boundary condition is set up when adatoms diffuse at the boundaries.

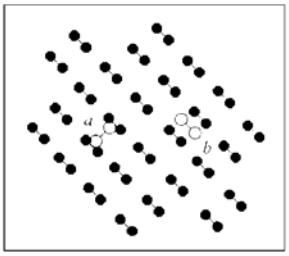

FIG. 1 Ad-Dimers on Si(100) Surface
a indicates the bond of ad-dimer is perpendicular to the substrate dimer rows in the 2×1 reconstruction, while *b* indicates that of the same ad-dimer is parallel to the substrate. The orientation shown in *a* is more stable. The black circles are the substrate dimers in the 2×1 reconstruction, and the white circle denotes the Si dimer adsorbed on the substrate.

3 Results and Discussion

3.1 Nano Si Wires Growth on Si(100) Surface

A typical simulation image of 1D nano Si wires grown on Si(100) is shown in Fig. 2, which resembles the STM experimental image closely[1,15]. The growth conditions are set to the deposition flux $F = 10^{-3}$ ML/s, total coverage $\theta = 0.1$ ML and surface temperature $T = 500$K. The migration barriers of Si adatom are 0.7eV along the dimer rows and 1.0 eV across the rows, respectively[6]. So the diffusion of Si adatom along the dimer rows is 1047 times faster than that across the rows at this substrate temperature, which is a highly anisotropic diffusion. According to the experimental data measured from the anisotropic growth of Si on Si(100) surface[14], the ratio of sticking at end site is approximate 50 times more than that at side site and is independent of the island length during the growth. The probabilities for adatoms to form perpendicular and parallel dimers are given to be 0.8 and 0.2, respectively. These anisotropic conditions of diffusion and sticking are effective in the simulation of the 1D Si wires' growth on Si(100) surface.

It can be seen clearly from Fig. 2 that particularly straight dimer-row islands with high shape anisotropy are formed on the Si(100) surface, which are perpendicular to the dimer rows of the substrate. There are few parallel dimers on the substrate. It is known from the observation on the dimer formation and wires growth that the dimers (including perpendicular and parallel) form at very low coverage, and then the perpendicular wires grow while the parallel dimers disappear gradually, at the same time more and more adatoms deposite and stick to them. It is puzzling that the growth of 1D Si wires is perpendicular to the direction of fast diffusion, which is contrary to our expection. Several models have been proposed to explain this surprising growth feature[15—17]. Our simulation results also indicate that the shape anisotropy of islands is mainly caused by

FIG. 2 Typical Simulation Image of 1D Si Wires' Growth on Si(100) Surface

anisotropic sticking rather than by anisotropic diffusion. Even if we set the growth conditions to be perfect anisotropic diffusion (1D diffusion along the dimer rows) and isotropic sticking, no 1D wires would grow. The average length of these 1D Si wires is 16 atoms at the surface temperature T= 500K, as shown in Fig. 2.

To gain an insight into the growth feature of Si on Si (100) surface, the anisotropic diffusion and growth are simulated at various substrate temperatures and the average lengths of islands in these cases are measured. The temperature dependence of the average length is shown in Fig. 3, where the growth conditions are same as what in Fig. 2. We also assume that the ratio of sticking probabilities at end site is 50 times higher than that at side site and is independent of the substrate temperature. The average length of islands increases with the temperature increasing. The larger diffusion rate means a higher probability of an arriving adatom to find an existing island before another adatom is deposited to provide a chance for nucleation, giving a rise in lower island density and larger average length. On the other hand, the deposition flux can also affect the island density and its length. To obtain longer Si wires, we can decrease the deposition flux, while the surface temperature is invariable. The lower deposition flux means the less adatom diffusion simultaneous on the substrate, yielding the lower island density and larger average length at the same surface temperature.

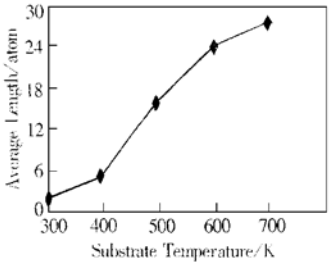

FIG. 3　Temperature Dependence of Average Length of Si Wires
The deposition flux F= 10^{-3}ML/s and total coverage θ= 0.1ML.

3.2　Nano Al Wires Growth on Si(100) Surface

Diffusion and growth of Si on Si(100) surface have been studied intensively. However, little is known about that of the metal on Si(100) surface. The diffusion and growth of Al on Si(100) surface are also simulated by using the model mentioned above. The Al adatom has smaller binding energy and longer bonds to the Si substrate than Si adatom, and the diffusion barriers for Al on Si(100) are 0.3 and 0.1eV along and across the dimer rows respectively[18]. This means that Al adatoms diffuse across faster than that along the dimer rows of the Si substrate, which is contrary to the behavior of Si on Si(100) surface. The diffusion of Al adatom across the dimer rows is 2283 times faster than that along the rows at the temperature T= 300K, which is also a highly anisotropic diffusion. To reflect the experiments of low-coverage Al form the perpendicular 1D islands on Si(100) surface, the probability of Al adatoms to form the perpendicular dimers P= 1 and perfect anisotropic sticking are presented in our simulation model. It means that all dimers are formed perpendicular to the dimer rows and the Al adatoms can stick only to the ends of the islands but not the sides. The topology of the energy surfaces shows[18] that the size of Al atom is larger than that of Si atom in the substrate and can form bonds at the position on or between the dimer rows of the substrate. The positions that are perpendicular to the dimer

rows have almost the same energy. So it is reasonable to say that the perpendicular direction of the substrate is beneficial to Al adatoms' diffusing and sticking.

Typical image of 1D Al wires grown on Si(100) surface is shown in Fig. 4, where $F = 10^{-3}$ ML/s, $T = 300$K and total coverage $\theta = 0.1$ML. This image confirms the experiments.[19] The average length of islands is 25 atoms, which is larger than that of Si growth on Si(100) surface at $T = 500$K. The above results show that long 1D Al wires can grow more easily than Si wires on Si(100) surface because of the lower diffusion barriers and the higher diffusion rate of Al adatoms. The average length of Al wires increases with the increasing temperature or the decreasing deposition flux, as is similar to that of Si wires growth. On the other hand, with the coverage increasing, coalescence will occur. The wires become longer and longer, and 2D islands growth will also take place. To get high-quality 1D nano wires, the growth conditions, such as surface temperature, deposition flux and coverage, should be optimized, and the high quality substrate should be prepared as well.

FIG. 4 Low Coverage Al Formed Perpendicular 1D Islands on Si(100) Surface

4 Conclusion

The growth of nano Si and Al wires on Si(100) surface is simulated by Monte Carlo method, where the anisotropic diffusion and anisotropic sticking are under consideration. It is shown that the shape anisotropy of islands is mainly caused by anisotropic sticking rather than by anisotropic diffusion. Although the situations of diffusion of Si and Al on Si(100) surface are different, i. e., it is faster for Si adatoms to diffuse along the dimer rows than across the rows, while as is contrary to Al adatoms, they can form the similar 1D wires because of the anisotropic sticking. Of course, ideal growth substrates are assumed in our simulation model, clean, big, smooth enough and no defects such as steps or kinks on. A complete model should include deposition, diffusion, nucleation and coalescence effects, as well as substrate temperature, substrate defects and sticking anisotropy. The influence of the deposition flux, the coverage, and the temperature windows on the optimum growth of 1D nano wires will be investigated further.

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