USING MOLECULAR DYNAMICS SIMULATION TO STUDY THE GROWTH OF GE THIN FILM ON SI SUBSTRATE

SỬ DỤNG PHƯƠNG PHÁP ĐỘNG LỰC HỌC PHÂN TỬ NGHIÊN CỨU SỰ PHÁT TRIỂN CỦA MÀNG MỎNG GE TRÊN CHẤT NỀN SI

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Abstract - Molecular dynamics simulations were conducted to investigate Ge thin film growth on Si substrates. The growth mode, surface morphology, and the layer coverage ratio of Ge atoms were investigated. The surface of the Ge thin film is not smooth, voids and vacancies are highly formed as the incident energy is lower than 0.1 eV. The Ge thin film grows by a layer-by-layer mode as the incident energy is raised from 0.1 eV to 0.3 eV. When the incidence energy is raised from 0.5 eV to 1.0 eV, film mixing is seen as a result of the incident atoms penetrating into several of the substrate layers. As the incident energies are raised to 10.0 eV, the sputtering mode is observed. As the temperature of the Si substrate rises from 300 K to 1000 K, under the incident energy of 0.1 eV, the layer-by-layer growth mode is still maintained, and the surfaces of the coating are quite smooth. The temperature of the Si substrate increase, and the layer coverage ratio of Ge atoms increases.

Key words - Deposition; Germanium; Silicon; Molecular Dynamics

Tóm tắt - Các mô phỏng động lực học phân tử được thực hiện để khảo sát sự phát triển màng mỏng Ge trên chất nền Si. Chế độ tăng trưởng, hình thái bề mặt và tỷ lệ bao phủ lớp nền của các nguyên tử Ge được nghiên cứu. Khi năng lượng tới của nguyên tử lắng đọng thấp hơn 0,1 eV thì bề mặt của màng mỏng Ge không phẳng, hình thành nhiều khoảng trống trong lớp phủ. Màng mỏng Ge phát triển theo chế độ từng lớp khi năng lượng tới tăng từ 0,1 eV đến 0,3 eV. Khi năng lượng tới được tăng từ 0,5 eV đến 1,0 eV, sự trộn lẫn giữa lớp phủ và chất nền xảy ra do các nguyên tử tới thâm nhập vào một số lớp chất nền. Khi năng lượng tới được tăng lên 10,0 eV, chế độ phún xạ được quan sát thấy. Khi lắng đọng với nhiệt độ của chất nền Si tăng từ 300 K đến 1000 K, năng lượng tới của nguyên tử lắng đọng 0,1 eV, chế độ tăng trưởng từng lớp vẫn được duy trì và bề mặt của lớp phủ khá phẳng. Nhiệt độ của chất nền Si tăng dẫn đến tỷ lệ bao phủ lớp nền của các nguyên tử Ge tăng lên.

Từ khóa - Lắng đọng; Gecmani; Silic; Động học phân tử

1. Introduction

Ion-beam-assisted deposition (IBAD), a popular method for creating thin films on substrates for additional applications, uses reactive or inert gas ions [1]. The IBAD method could be used in two ways to create a thin film. One is to encourage the growth of the film and improve the mobility of the deposited atoms. The other involves bombarding a solid substrate's surface to strip its atoms away in preparation for further deposition. The ion incident energy, ion incident angle, and substrate temperature must all be adjusted in order to have these two application-specific characteristics. The quality and morphology of the deposited thin film will be impacted by these IBAD process parameters. The epitaxy [2] and the film mixing [3], which indicate the mixing of the deposition atoms and the substrate atoms, have prevailed at lower energies under the various combinations of IBAD process parameters. Sputtering [4], a process in which the incident atoms remove substrate atoms, is a phenomenon that may be created at greater energies.

Since Si/Ge superlattices and heterostructures have superior electrical and optical characteristics, they are in high demand for the production of optoelectronic devices such as ultrafast photodetectors, solid-state lasers, photodiodes, etc. [5-9]. However, the quality of these materials with customized properties is significantly influenced by film growing procedures [10].

Therefore, studying the effect of parameters on the deposition of Ge atoms on Si substrate is necessary. In this study, we study the influence of incident energy and substrate temperature on the quality and morphology of Ge thin film.

2. Methodology

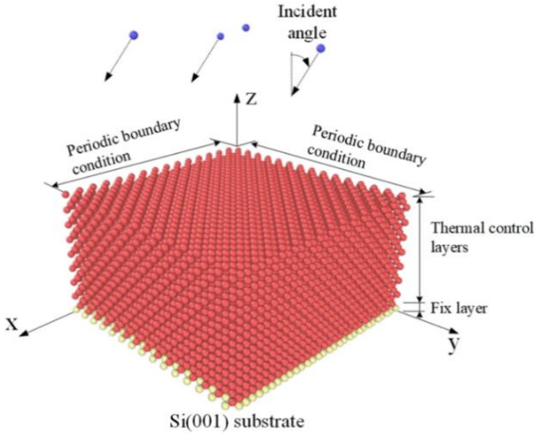


Figure 1. *Simulation model for the deposition of Ge atoms on Si substrate*

A simulation model for the deposition of Ge atoms on Si substrate was presented in Figure 1. The substrate is composed of 15a x 15a x 8a, with a is the lattice constant of Si. The layer at the bottom is fixed to provide structural stability of the substrate during deposition. The temperature of the substrate is managed by the thermostat control layers.

To limit the effect of model size, periodic boundary conditions are applied in the *x*- and *y*- directions. In this study, Ge incident atoms were deposited at a deposition rate of 2 atoms/ps. The velocity of Ge atoms is calculated based on incident energies from 0.01, 0.1, 0.3, 0.5, 1.0, to 10 eV. The incident angle in this study is chosen 0^0.

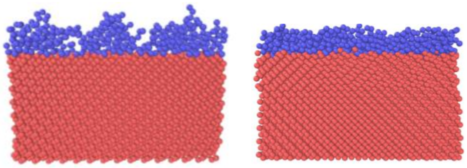
The Tersoff potential [11] was used to specify the interactions between Ge-Ge, Ge-Si, Si-Si atoms. All MD simulations were conducted by the large-scale atomic/molecular massively parallel simulation (LAMMPS) [12]. To visualize and evaluate the simulation results, we used OVITO software [13]. The parameters used in the deposition process are shown in Table 1.

Table 1. *Parameters for specimens used in the deposition process*

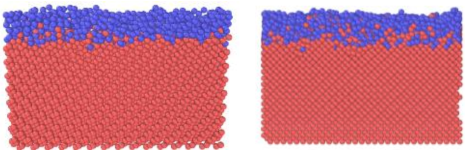
Material	Substrate: Si atoms	Incident atoms:Ge
Dimensions	15a x15a x 8a	
Number of atoms	14850	3000
Ensemble	NVE	
Time step (ps)	0.001	
Incident energies (eV)	0.01, 0.1, 0.3, 0.5, 1, 10	
Temperature (K)	300; 500; 750; 1000	

3. Results and discussion

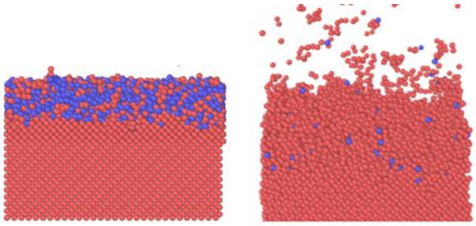
3.1. Effect of incident energies



(a) 0.01 eV – 300 K (b) 0.1 eV – 300 K



(c) 0.3 eV – 300 K (d) 0.5 eV – 300 K



(e) 1.0 eV – 300 K (f) 10.0 eV – 300 K

Figure 1. *The morphology of substrate under the deposition process at temperature 300 K with different incident energies: (a) 0.01 eV, (b) 0.1 eV, (c) 0.3 eV, (d) 0.5 eV, (e) 1 eV, (f) 10 eV*

Figure 2 shows the morphology of substrate under the deposition process at temperature 300 K with different incident energies: (a) 0.01 eV, (b) 0.1 eV, (c) 0.3 eV, (d) 0.5 eV, (e) 1 eV, (f) 10 eV. The results show that the surface of the Ge thin film is not smooth, voids and vacancies are highly formed. These events could be explained by the low incidence energy, where the incident atoms have poor atom mobility and are unable to move energetically. These phenomena could be seen when the film grows in the Volmer-Weber mode [14]. The surface is smooth when the incident energy is raised from 0.1 eV to 0.3 eV, as shown in Figure 2(b-c); Because the incident atoms' energy is sufficient to fill the voids and they have superior thermal diffusion or mobility. Additionally, in the Frank-van der Merwe mode, when the atom mobility is advantageous, the film is grown layer by layer [14]. As seen in Figure 2(d-e), when the incidence energy is raised from 0.5 eV to 1.0 eV, film mixing is seen as a result of the incident atoms penetrating into several of the substrate layers. As the incident energies are raised to 10.0 eV, the sputtering mode is observed due to the kinetic of incident atoms being so high, as shown in Figure 2(f).

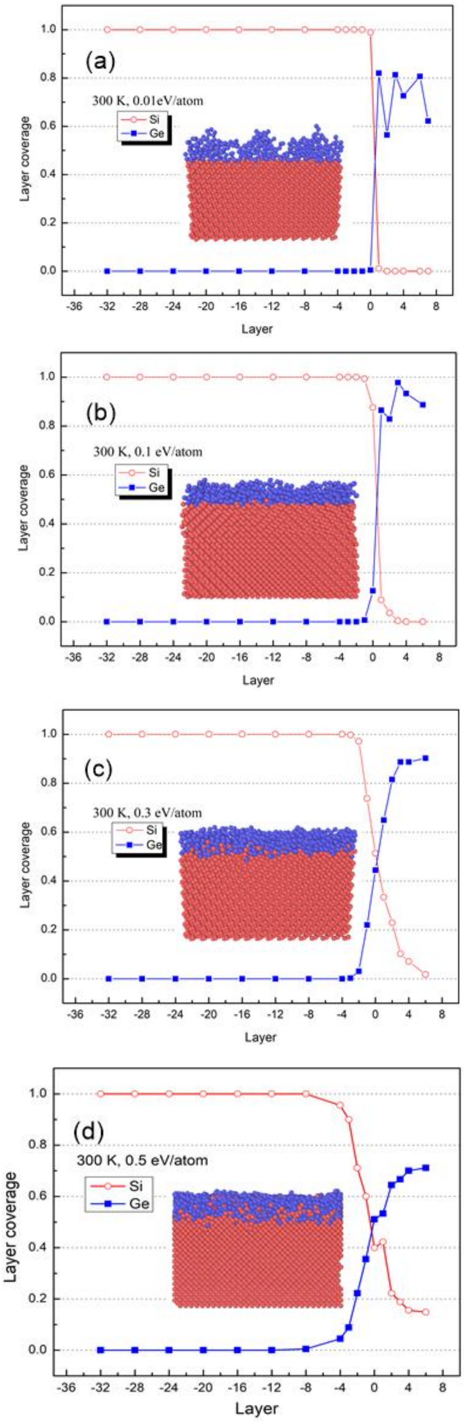
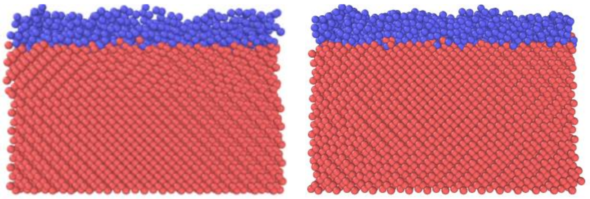


Figure 3. *Fraction of atoms along z- direction after deposition of 3000 Ge atoms on Si substra*

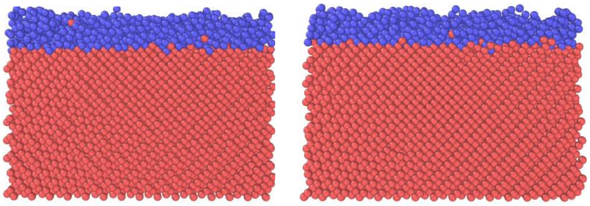
Figure 3 illustrates the distribution of Ge and Si atom numbers in intervals in the *z*-direction at the final state to better characterize the intermixing phenomena. The red line shows the ratio of Si atoms of the current layer to a standard layer, and the blue line presents the ratio of Ge atoms of the current layer to a standard layer. The initial surface of the Si substrate is defined at layer 0. The bottom layers of the substrate keep the structure stable due to being unaffected by incident atoms. Some of the substrate atoms near the surface diffuse into the deposited Ge film, and some Ge atoms penetrate the substrate. Figure 3(a) shows that the diffusion of the substrate into the Ge deposition surface is very little, and the filling ratio of the Ge atoms is low due to the low incident energy leading to the appearance of a lot of voids and vacancies. When the incident energy is between 0.1 eV and 0.3 eV, diffusion occurs in several layers at the surface of the substrate. Furthermore, the filling ratios of the incident Ge atoms are relatively high, indicating the possibility of layer-by-layer growth taking place in this incident energy range. When the incident energy reaches 0.5 eV, the diffusion process occurs strongly. As shown the ratio of Ge atoms on the surface is low and the percentage of Si atoms diffused into the Ge film is quite high, as shown in Figure 3(d). The results show that in the incident energy range from 0.1 eV to 0.3 eV, the deposition surface achieves good smoothness, and layer-by-layer growth is observed. This demonstrates that, as incident energy increases, intermixing may take place deep beneath the substrate's top layer. This result is consistent with experimental result [15] and some simulation studies [6, 16].

3.2. Effect temperature

In this section, to study the effect of temperature on the growth of Ge thin film on Si substrate, the deposition processes are conducted at incident energy 0.1 eV with various temperatures: 300 K, 500 K, 750 K, and 1000 K.



(a) 300 K (b) 500 K



(c) 750 K (d) 1000 K

Figure 4. *The morphology of substrate under the deposition process at incident energy 0.1 eV with various temperatures: (a) 300 K, (b) 500 K, (c) 750 K, (d) 1000 K*

The morphology of thin film under the deposition process at incident energy 0.1 eV with various temperatures is shown in Figure 4. The results show that when the temperature increases from 300 K to 1000 K, the layer-by-layer growth mode is still maintained, and the surfaces of the coating are quite smooth. To evaluate the intermixing phenomenon and the quality of the Ge coating, the layer coverage ratio of Ge atoms along the z-direction after deposition of 3000 Ge atoms on Si substrate under different temperatures is shown in Figure 5. It points out that as the temperature of the Si substrate increase, the layer coverage ratio increases. Ge atoms can even pierce the substrate layer at high substrate temperatures. This indicates that when the substrate temperature is high enough, mixing can take place beneath the top layer of the substrate.

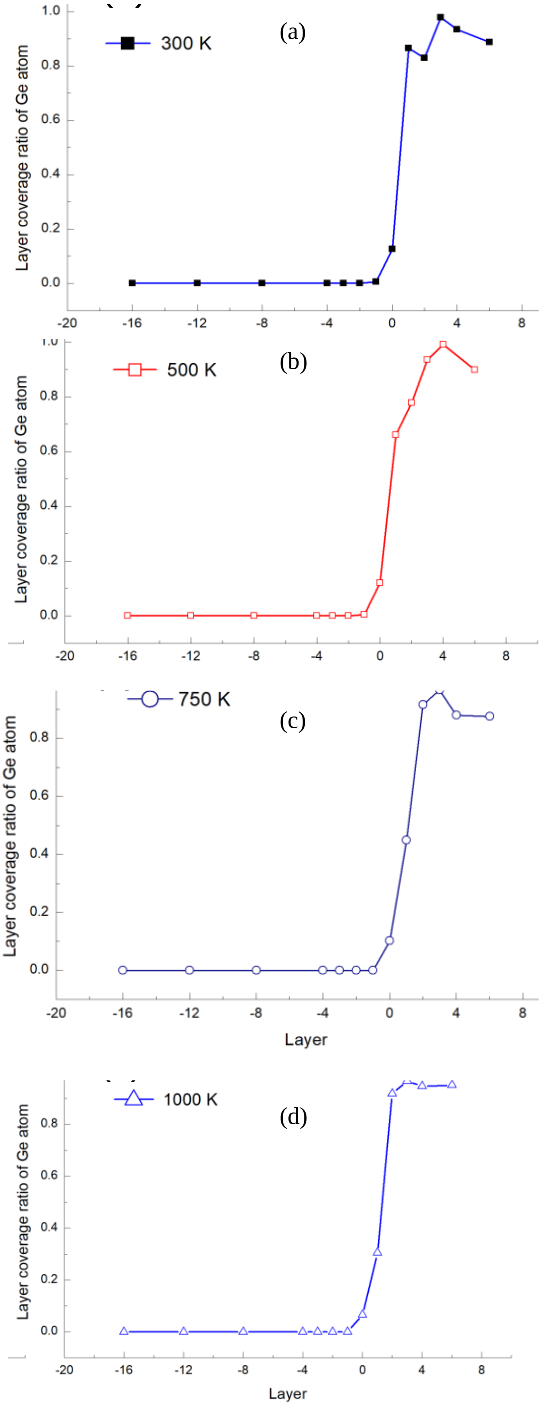


Figure 5. *The layer coverage ratio of Ge atoms along z- direction after deposition of 3000 Ge atoms on Si substrate under different temperatures*

4. Conclusion

We study the effect of the incident energy of the Ge atom and the temperature of Si substrate on the growth of Ge on Si substrate using molecular dynamics simulations. As the incident energy is lower than 0.1 eV, the surface of the Ge thin film is not smooth; Voids and vacancies are highly formed. The surface is smooth when the incident energy is raised from 0.1 eV to 0.3 eV because the incident atoms' energy is sufficient to fill the voids and they have superior thermal diffusion or mobility. When the incidence energy is raised from 0.5 eV to 1.0 eV, film mixing is seen as a result of the incident atoms penetrating into several of the substrate layers. As the incident energies are raised to 10.0 eV, the sputtering mode is observed due to the kinetic of incident atoms being so high. As the temperature of the substrate rises from 300 K to 1000 K, the layer-by-layer growth mode is still maintained, and the surfaces of the coating are quite smooth. The temperature of the Si substrate increase, and the layer coverage ratio of Ge atoms increases.

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