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Molecular-dynamics simulation of germanium film growth by cluster deposition

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Abstract

Ge films have been grown by depositing Ge-atom clusters with different initial energies on Si(0 0 1) substrates with molecular-dynamics simulations utilizing the Stillinger–Weber (SW) many-body potentials for Ge and Si. The structural properties and the stress distribution of the films have been characterized. We find that the films formed by depositing the clusters with higher initial energies have better qualities and the stress values in such films are a little higher. We have also compared the stress value with the experimental data. In addition, we find that the stress distribution is more gradual throughout the system in the case of higher cluster energy.

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Keywords: Ge films; Cluster deposition; Molecular-dynamics simulation; Stillinger–Weber potential; Stress

1. Introduction

Depositing Ge on Si substrate has been of great interest in the last decades, because epitaxial and nanocrystalline films, both of which are important semiconducting materials, can be formed during the deposition process. Ge epitaxial layers on Si can be used as high performance photodetectors and heterojunction dipolar transistors [1,2]; the islands formed during Ge/Si growth can be used for the direct fabrication of quantum dots (QDs), which are promising candidates for optoelectronic applications [3].

During Ge film growth, the stress caused by the large lattice mismatch (4.2% between Ge and Si) plays an important role and makes the film grow in the Stranski–Krastanow (SK) mode: initial two-dimensional (2D) growth lasts till several

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epitaxial layers are formed, then the film's surface roughens to relax strain and finally islands appear on the surface [4]. Actually the pathway for the relaxation is rather complicated and still under study [4–6]. Real-time stress measurement has been taken to investigate this process [7,8]. On the other hand, the residual stress in the prepared film modifies the electronic structure of Ge/Si. Experimental studies have been carried out to improve Ge/Si film's properties by controlling the stress in it [1].

Compared with the progress in the studies on measuring and controlling the stress in Ge/Si, few researches in this field have been reported. In the present work, Ge/Si films are prepared by depositing Ge-atom clusters with different energies on Si(0 0 1). The structural properties and the stress distribution of the films are analyzed to estimate the influence of cluster energy. Cluster beam deposition (CBD) is chosen as the method to prepare the films, because this method is simple and valid to generate Ge nanocrystalline films [9,10] and may be important in the further researches. The details of CBD method can be found in the literatures [10,11].

2. Computational details

In the simulation, Newton's equations of motion are integrated with the Verlet algorithm [12] at a constant time step of 0.005 ps for the collision of the deposited atoms and the substrate. The time step is larger than those usually used [13,14], which may reduce the accuracy of the calculation. We have performed two simulations with different time steps 0.005 and 0.001 ps to check for the effect. The two sets of simulations produced similar structures and stress values of the deposited films. So the time step 0.005 ps is acceptable in our work. The interatomic potential for silicon is due to Stillinger and Weber [14]. This potential involves both two- and three-body terms and has been proved to give a good description of the equilibrium properties of silicon in the crystalline, liquid and amorphous phases. Appropriate parameters for Ge–Ge and Si–Ge interactions have been chosen according to the literatures [14,15].

We construct a silicon crystal as the substrate, which is 12 ML thick, with its (0 0 1) face toward the vacuum. Each monolayer contains 144 atoms. The surface of the crystal has an area of $6\sqrt{2}a_0 \cdot 6\sqrt{2}a_0$, a_0 being the lattice constant. The X-axis is along [1 1 0] and the Y-axis perpendicular to it. Initially, the grid origin is located in the top layer of the crystal. Periodic boundary conditions are applied in the XY plane and the system is open along the Z-axis. During the total simulation process, the atoms of the two layers in the bottom are held fixed in their initial positions and the two layers immediately above them are held at a mean temperature of 1000 K by scaling the velocities of the atoms in them every ten steps. Before depositing clusters, we modify the positions of the atoms in the four layers close to the substrate surface using the data given by Balamane et al. [16] for the displacements of the atoms of a $2 \times 1(0\,0\,1)$ surface; Maxwellian velocity distribution is chosen for the velocities of all the movable atoms. Subsequently, the slab is thermalized at 1000 K for 25 ps.

Ge_{12} clusters are introduced into the system one by one till six layers of atoms are deposited. To the best of our knowledge, the ground-state structure of Ge_{12} cluster has seldom been investigated by modeling studies utilizing the SW potential to simulate the interaction of atoms, and on the other side those possible structures of Ge_{12} cluster produced by the quantum method are not proper to introduce into our work mechanically for the two different methods tend to produce different results in this research filed [16]. As an approximation, we treat the cluster as a fragment of the amorphous Ge produced by quenching [17], like some researchers have done in the deposition of Si-atom clusters [18,19]. In each case, the deposition rate is one cluster deposition every 5000 time steps (25 ps). The lateral starting point for a cluster is chosen randomly and the height of its mass center is chosen to ensure there is no interaction between an atom in it and one on the substrate. The atoms in clusters have initial velocities perpendicular to the surface of the substrate. To investigate the influence of cluster energy on the film's quality and the stress distribution, three films are prepared by depositing clusters with different initial energies (1, 4 and 10 eV/atom), respectively.