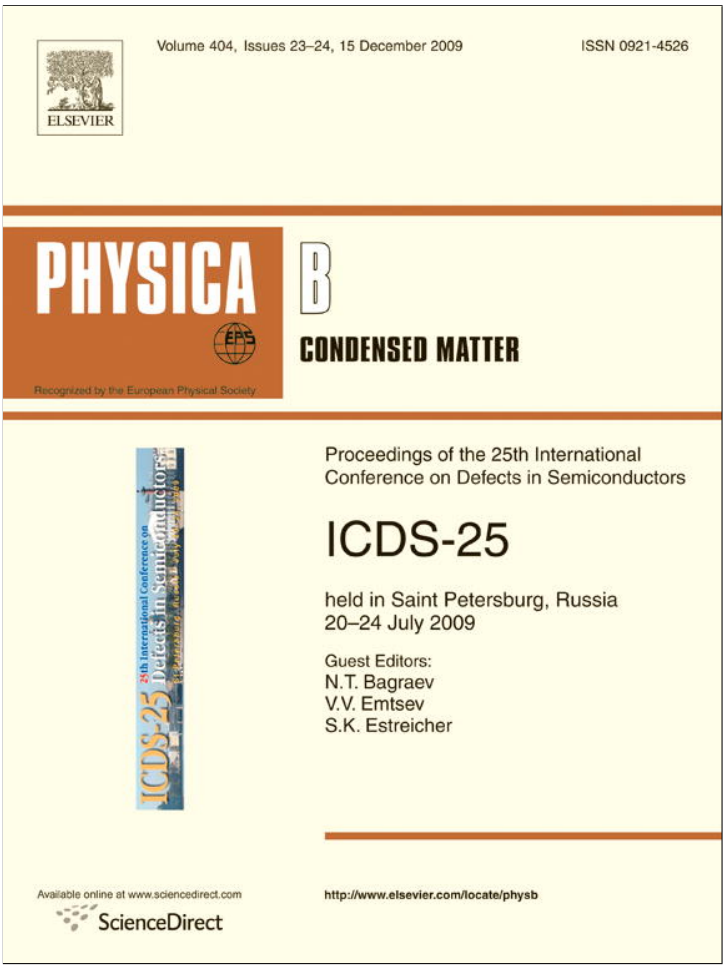

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Stress-induced nanoislands nucleation during growth of Ge/Si heterostructures under low-energy ion irradiation

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ABSTRACT

Stress-induced nucleation of nanoislands under pulsed low-energy ion-beam assisted growth of Si/Ge heterostructures is studied by molecular dynamics and Monte-Carlo calculations. It is shown that cluster of interstitials is produced in Si bulk by an ion impact. Stresses induced at the surface by clusters of interstitials affect migration ability, stimulating nucleation and growth of Ge nanoislands. The main effects of ion-beam action observed in experiments, e.g. increase in islands density, decrease in islands average size and nonmonotonous dependence of islands density upon degree of molecular beam ionization, are interpreted in terms of stress-induced mechanism.

1. Introduction

Ge/Si heterostructures containing dense and homogeneous arrays of quantum dots (QD) attract the attention of researchers, working both in basic and in application fields [1,2]. Low-energy ion-beam assisted deposition takes an advantage of molecular beam epitaxy combined with low temperature processing [3]. This method, which is still under development, is receiving increasing attention and holds promise for the effective control over self-organized QD array growth. Despite a long-term study of the ion-beam assisted deposition still there is a lack in understanding of the elementary processes which occur on the atomic scale during an ion impact in ps range of time. Molecular dynamics (MD) [4] is a powerful simulation tool, which may give an insight into the microscopic mechanism of ion-beam action. On the other hand, Monte Carlo (MC) simulation [5] provides an adequate description of growth process in a longer time range comparable with that in the experiment.

In this work we present joint MD and Monte Carlo simulation study of interstitials introduced into Si bulk by ion impinging and their role in producing surface stresses in Ge/Si heterostructure and stress-induced formation of Ge islands.

2. Experiment

The samples were grown on a molecular-beam epitaxy setup equipped with a germanium molecular ion source [4,6]. The samples were prepared through the conventional molecular-beam epitaxy of germanium on the Si(1 0 0) surface and the molecular-beam epitaxy with pulsed irradiation by a beam of low-energy Ge^+ ions. The angle of ion beam incidence to the surface normal was 52.3°. Twist angle of ion beam incidence relative to wafer (1 1 0) direction was 18°. The ion energy could be controllably varied from 50 to 250 eV. The pulsed irradiation (with the pulse duration ~0.5 s) was performed after the deposition of each germanium monolayer (ML) was completed. The structures were grown at a deposition rate of approximately 0.1 ML/s and at the temperatures of the substrate 570–670 K. In all experiments, the total amount of deposited germanium was identical and equal to 5 ML. The morphology of the surface was in situ examined by scanning tunneling microscopy (STM). The samples were studied at room temperature in a constant tunneling current mode.

3. Molecular dynamics study

MD calculations included 20 ML of Si(1 0 0) structure covered with 1 ML of Ge arranged in (2×1) reconstructure. The lateral sizes of the mesh were $5.43\,\text{nm} \times 5.43\,\text{nm}$ with periodical boundary conditions implied in lateral directions. The interaction between the atoms was expressed by Tersoff potential [7]. To avoid the influence of initial atoms positions, the system was allowed to relax during 1 ps at 350 °C, and the obtained configuration was taken as the initial one. Then a Ge atom moving from the height of 0.5 nm towards the surface was added to the system. The atom kinetic energy was 150 eV. The angle between the velocity vector and the normal to the surface was 52.3°. Twist angle between the impacting atom velocity and the

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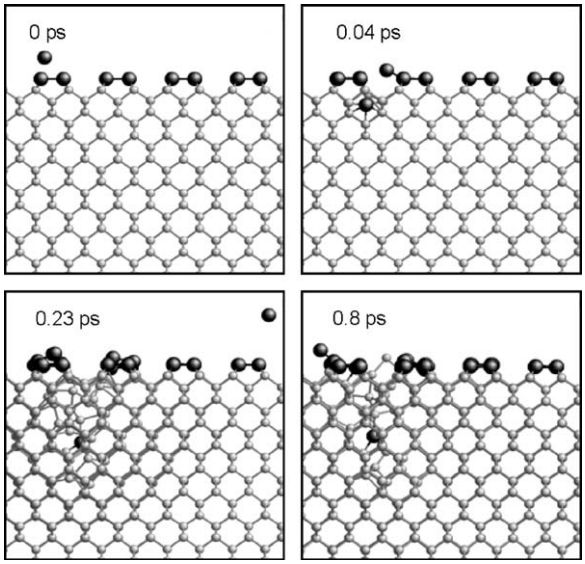

Fig. 1. Evolution of Ge/Si(1 0 0)-(2×1) system at different times after an ion impact, obtained by MD calculations. Ge atoms are painted in black, Si atoms—in gray. In orientation presented interstitials are well-marked as an atoms located inside hexagonal cells.

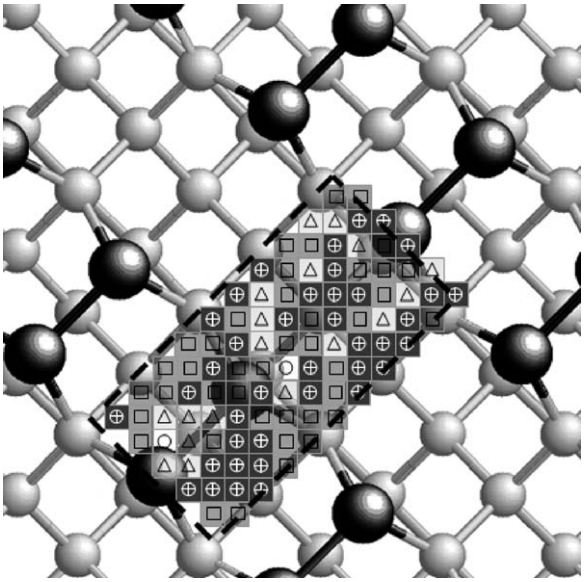

Fig. 2. Cross section for the processes induced by a Ge atom hitting a Ge/Si(1 0 0):(1×2) surface. Different colors and symbols are used to distinguish between different numbers N_{def} of interstitials formed. O (white): $4\le N_{def}\le6$, Δ (light gray): $7\le N_{def}\le9$, □ (dark gray): $10\le N_{def}\le11$, + (black): $12\le N_{def}\le14$. Approximately, a halve of interstitials is created in the bulk.

dimmer rows was taken equal to 18° and 72° (which corresponds to geometry of the experiment for (2×1) and (1×2) surface reconstructures, respectively). MD calculations were performed for the set of initial (x,y) positions of Ge ion within the elementary cell of (2×1) surface. The process modeled by each MD simulation took approximately 0.8 ps. This time was found to be long enough for the formation of stable defects (some simulations were prolonged for 20 ps with no further defect evolution observed).

4. Results and discussion

Fig. 1 presents the sequence of snapshots made at different time steps of a typical impinging process as simulated by MD calculations. The main elementary processes induced by an ion impact are: ion recoil, sputtering, displacement of Si and Ge atoms, formation of Ge and Si interstitials and vacancies. The detailed analysis showed that the quantitative characteristics of each process strongly depend upon the position in which an ion hits the surface. In order to make the averaging over the surface we divided an elementary surface cell into 100 sections and performed simulations, varying an ion initial (x,y) positions within the elementary cell. Finally, we were able to build the cross section displayed in Fig. 2. Events can be divided into four main categories, differing one from another by the number of vacancy/interstitial pairs generated by the impact. The analysis has shown that in average 10.2 interstitials are formed per an impact, and approximately 5 ones are created in Si bulk. Their depth is distributed in interval [1; 14] ML and the average depth is equal to 5 ML.

5. Monte Carlo modeling

Since all the elementary processes studied by MD simulations are random events, the statistical aspect should be taken into account in order to understand the film growth. For that reason we implied the results of MD simulations to Monte Carlo (MC) modeling, using the model developed in the previous works [5,6].

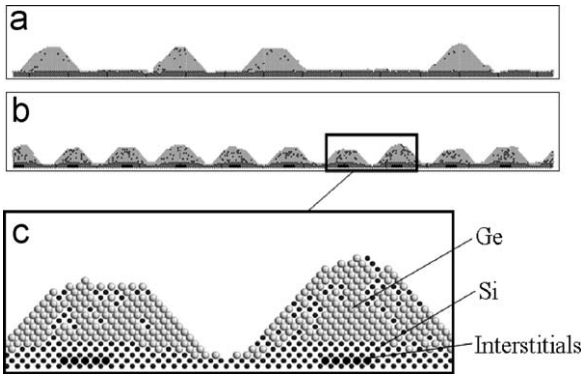

Fig. 3. (a,b) Calculated surface morphologies according to the results obtained from the simulation of deposition of five germanium monolayers at the temperature of the substrate $T=620$ K for the following cases: (a) conventional molecular-beam epitaxy, (b) molecular-beam epitaxy with generation of clusters of interstitial atoms (10 clusters, each containing five interstitial atoms and located at depth of 5 ML). (c) Fragment of calculated structure for the case presented in panel (b).

The details of the model are described elsewhere [6]. Here we just mention the main assumptions of MC model. The growth process is simulated through the sequence of Ge atoms deposition and diffusion hops of Ge and Si atoms. The probability of a hop from specific position depends on the number of atoms in local environment and on the local stresses. Stresses are induced both by Ge/Si crystal lattice mismatch and by interstitials embedded in the bulk of heterostructure. Interstitials are generated by ion impacts. The stresses are regularly recalculated during the heterosystem evolution using the conjugate-gradient method of the elastic energy minimization [8]. In order to avoid dramatic escalation of computational time under the joint solution of kinetic and elastic problems, two-dimensional square lattice was considered with (11) surface orientation. According to the results of MD the number of interstitials per ion impact was put equal to

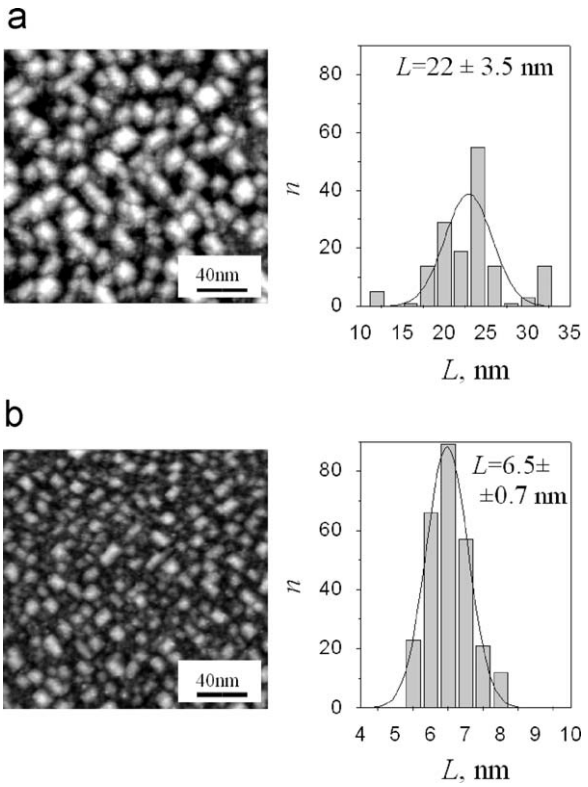

Fig. 4. (a,b) STM images (200×200 nm) of the surface with three-dimensional islands formed after deposition of five germanium monolayers on the Si(1 0 0) substrate and corresponding size distributions of islands (n is the number of islands) for two types of experiments: (a) conventional molecular-beam epitaxy of germanium on the Si(1 0 0) substrate and (b) molecular-beam epitaxy with pulsed irradiation by Ge^+ ions. Conditions: the molecular germanium flux density is $7 \times 10^{13}\,cm^{-2}\,s^{-1}$, the temperature of the substrate is $T = 620$ K, the ion beam energy is $E = 140$ eV, the pulse duration is $= 0.5$ s, and the ion flux density is $I = 3.1 \times 10^{11}\,cm^{-2}\,s^{-1}$.

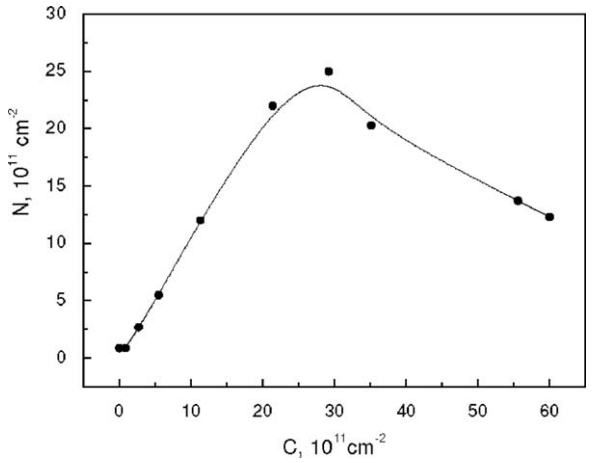

Fig. 5. Calculated dependence of the density of three-dimensional islands on the density of clusters generated by the ion beam for the case of molecular-beam epitaxy which composed of five interstitial atoms and located at a depth of 5 ML from the initial surface.

5. All interstitials were assumed to be motionless and generated in Si bulk, namely, 5 ML below Si/Ge interface.

Results of MC modeling are presented in Fig. 3. Ge atoms are painted in light gray, Si atoms in dark gray, interstitials in black. Formation of Ge islands under deposition without ion-beam action (Fig. 3a) can be explained in terms of stress-forced mechanism. Nanoislands are nucleated randomly on the surface of wetting layer as a local hillock. Since compressive stress in the Ge hillock is decreased, bond energy of adatoms is increased, stimulating the further growth of an island. Contrary to conventional MBE, nucleation of Ge islands under ion-beam action is no more random but predetermined in the regions of ion impact (Fig. 3b). Stretching stresses produced by interstitials cluster embedded in the bulk turn out to be high enough. This results in dramatic rise of bond energy of Ge adatoms and, hence, nucleation and growth of an island. The strain-force mechanism works in the opposite direction in the regions between Ge islands, where both Ge and Si are intensively removed from Fig. 3c. MC simulation gives about 2.5 times higher density of Ge islands in the array under an ion-beam action (Fig. 3b), as compared to conventional MBE (Fig. 3a). This result is found to be in a qualitative agreement with STM data presented in Fig. 4. Islands density estimated from STM is 6.8×10^{11} and $\sim 2 \times 10^{11}\,cm^{-2}$ under and without pulsed ion-beam irradiation, respectively. Since Ge desorption is neglected in MC model, the higher islands density should lead to their smaller size (for the same amount of Ge deposited). This result of MC simulation (Figs. 3a,b) is confirmed by STM data (Fig. 4). The average size of the islands obtained in experiment is 6.5 nm for irradiated structures and 22 nm for those grown by conventional MBE.

MC simulations were carried out for various degrees of molecular beam ionization. As illustrated in Fig. 5, island density depends nonmonotonously on ionization degree, first increasing with the ion flux, then going down. The increasing behavior is expectable and interpreted in terms of a higher density of sites favorable for nucleation of islands. The further decrease of induced interstitials clusters results in overlapping between regions of compression fields formed in a local environment of each cluster. The compression affects mobility of surface atoms, so that material is intensively removed from the region of compression. When the surface front reaches clusters their annihilation occurs. The annihilated clusters can no more play role of nucleation centers, and the island density decreases. The non-monotonous dependence upon ionization degree is observed in experiment. However, maximum position in the experimental dependence is shifted to lower ionization degrees in comparison with that shown in Fig. 5. We believe that this numerical disagreement can be eliminated to some extend by taking more accurate distribution of generated clusters over depth into account.

6. Conclusion

Using joint MD and MC simulation the role of interstitials clusters generated by low-energy pulsed ion-beam irradiation during Ge deposition on Si is studied. Stress-induced mechanism of Ge island formation is revealed. The experimentally observed nonmonotonous dependence of islands density upon ionization degree is qualitatively reproduced by MC simulation. The descendant part of the dependence is interpreted in terms of compression region overlapping, which favors defect annihilation.

Acknowledgments

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