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Surface reconstruction induced by a pulsed low-energy ion beam during Si(111) molecular beam epitaxy

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Abstract

The morphology and reconstruction of a vicinal Si(111) surface during Si molecular beam epitaxy (MBE) by reflection high-energy electron diffraction (RHEED) was investigated in conjunction with pulsed actions (0.25–1 s) by low-energy (80–150 eV) Kr^+ ions in the dose range of 10^{11}–10^{12} cm^{-2}. Ion pulsed action was found to increase RHEED specular beam intensity corresponding to the improvement of surface smoothness during MBE growth. The maximum intensity enhancement was found if the pulsed ion beam is turned on at a fractional surface coverage of $\theta \approx 0.8$ and the substrate temperature ca 400°C. It was revealed that ion beam pulsed action induces (5×5) to (7×7) superstructure phase transition. As the substrate temperature increases, the area of (7×7) reconstruction induced by ion beam action was found to expand, and reached a maximum at 400°C. Above this temperature the (7×7) reconstruction area tends to the value of common Si MBE without ion beam action. We present a simulation model of MBE growth, which includes surface reconstruction under low-energy pulsed ion beam action. It is suggested that the ion beam induced $(5\times5)\Rightarrow(7\times7)$ superstructure phase transition allows a decrease in the activation energy of adatom diffusion and improves the surface smoothness at Si MBE. The modeling results are in good agreement with the main experimental data at a different surface coverage, with the temperature of the substrate being the same for both single- and multi-pulsed ion beam actions. © 1999 Elsevier Science B.V. All rights reserved.

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1. Introduction

A major focus of research on nonequilibrium processes on a surface is the evolution of a surface morphology during thin film epitaxy. Crystal growth at a low temperature is probably the most attractive direction of studies on nonequilibrium surface processes partly due to the importance of interface structure to the synthesis of multilayer systems. The use of low-energy ion beams promotes crystal growth at extremely low temperatures where thermal beams would form amorphous material [1,2]. The kinetic energy of these ions is coupled directly to the growth surface facilitating local atomic rearrangement and allowing atoms to relax into perfect lattice sites. Details of the mechanism of energetic particle enhancement for low temperature epitaxy are not completely understood. In order to achieve a better understanding of ion beam induced changes in growth kinetics, it is worthwhile to study pulsed ion action under the layer-by-layer growth in con-

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junction with in situ control of the surface transformation.

Recently we investigated experimentally the growth of silicon layers under pulsed low-energy ion irradiation at different stages of growth according to the degree of filling of the surface atomic layer. To record the surface morphology in situ, we employed the method of reflection high-energy electron diffraction (RHEED) with observation of the specular intensity oscillations during two-dimensional layer growth of silicon [3]. We have found that a low-energy (~ 100 eV) Kr ion beam action of 0.25–1 s pulsed duration leads to increasing RHEED specular beam intensity during Si(111) molecular beam epitaxy (MBE) [4,5]. This corresponds to a decrease in the roughness of the growing surface. The effect of ion beam action was observed to strongly depend on the surface coverage (phase of RHEED oscillations), temperature of substrate and ion beam density. The subject of this study was to investigate the surface reconstruction under a low-energy ion beam pulse and to develop a model of MBE growth which includes the effect of surface reconstruction due to ion beam irradiation.

2. Experimental

The experiments were performed in an ultra-high-vacuum chamber with residual gas pressure $<10^{-8}$ Pa. The silicon wafers were 10 Ω cm B-doped Si(111) with orientation to within 0.1° according to X-ray diffraction data. The samples were cleaned by thermally removing the native oxide at 900°C. The Si deposition was done from an electron beam Si evaporator with a deposition rate of 0.05–0.2 biatomic layers per second. The buffer layer 200 nm thick was grown at 610°C followed by an annealing at 770°C to produce a flat surface with (7×7) reconstruction. To monitor in situ the evolution of the surface, the 15 keV RHEED intensity was measured with a camera. RHEED oscillation is a powerful in situ monitor for layer-by-layer growth during MBE. The oscillations commonly are described by evolution of surface step density [6–8]. By using a sufficiently low substrate temperature during Si MBE, the response of the RHEED oscillations is a rapid damping of both the amplitude and the average RHEED intensity level. This is explained by an increasing surface roughness, that is, multilayer growth, due to low adatom surface mobility, which results in an increased diffuse scattering of the reflected electrons. For intermediate substrate temperature very gradually decaying RHEED oscillations indicate layer-by-layer growth, where new islands are formed preferentially when the previous layer is almost completed. Increasing of the temperature allows reaching a state where the adatom surface mobility is sufficiently high for practically all adatoms to attain a terrace step edge. At this case the growth is controlled by step flow and there is no RHEED intensity oscillations. Our results concern mostly the intermediate temperature range.

The period of the RHEED oscillations was equal to the deposition time required to form a complete atomic layer. In the case of a Si(111) surface, a complete atomic layer is biatomic in thickness. The intensity was measured in Bragg diffraction conditions, which are very sensitive to any change in the surface morphology on account of the scattering of electrons, by the boundaries of steps, islands and surface defects. Under these conditions a unique correspondence is observed between the minimum of the surface roughness and the maximum of the intensity of the reflected beam.

The gas inlet system was installed in the vacuum chamber, and the gas flux was controlled by changing the slit width by an external electric field. Inside the vacuum chamber there were the units of gas ionization with electron strikes and ion acceleration by an applied voltage up to 200 V. The gas inlet system allows the formation the pulsed flux over 0.25 (the time lag to open the slit) to 1 s (the maximum level for keeping the vacuum after pulse action). Pure Kr gas was used in the experiments. The Kr ions hit the surface 54.5° off-normal direction. The ion current density was varied in the range of 0.1–0.6 μA cm^{-2}. With the pulse duration used in the experiments, the doses of a single pulse action were in the order of 10^{11}–10^{12} cm^{-2}. The experiments were performed at temperatures of 200–600°C.

3. Experimental results

First we studied a pulsed Kr ion beam action on an atomically clean Si(111) surface in the temperature range of 200–600°C. The RHEED intensity signal goes down when the ion beam switches on. After the pulse action the RHEED intensity goes up and tends to the initial value level. The difference in RHEED intensity before and after pulsed ion beam irradiation was found to increase as the ion energy grew or the substrate temperature decreased. This is consistent with the vacancy/adatom generation on the surface versus the ion energy and healing of defects at the annealing. The similar pulsed action with neutral Kr gas (no ionization) kept RHEED intensity practically the same as the initial value recorded for both the single and multi-pulse irradiation.

During Si MBE we have observed the known [8] RHEED intensity oscillations in the temperature range of 200–550°C. After deposition of one biatomic layer, the virgin (7 × 7) reconstruction transforms to the mixture of (7 × 7) and (5 × 5) superstructures [9]. Fig. 1 shows the RHEED oscillations at 400°C without ion beam and with ion beam induced changes for different surface coverage. The arrows in the Fig. 1b indicate the times at which the ion current pulse start to act. As the ion beam starts to act, the RHEED intensity goes down. The RHEED intensity strongly depends on a surface coverage θ after pulsed ion bombardment.

The ion beam induced intensity enhancement was found for coverages in the range $0.5 < \theta < 1$. There was practically no enhancement for the first half of the surface filling ($\theta < 0.5$). The maximum of intensity enhancement ΔI was found to be at $\theta = 0.8$ and ca 400°C. As the temperature went up to 500°C or down to 300°C the effect of ion beam action practically disappeared (see solid line in Fig. 2).

To clarify the observed effect, the pulsed ion beam actions were also performed immediately after interruption of Si deposition. In this case there was no RHEED intensity enhancement for any surface coverage. The ion beam switches on the RHEED intensity decreased and then recovered to the same level after pulse action. This

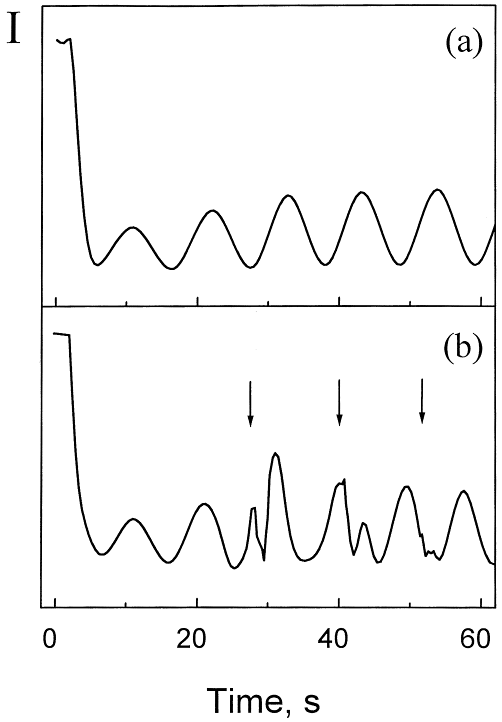

Fig. 1. RHEED specular beam intensity I versus time recorded during Si MBE on Si(111) at the substrate temperature of 400°C (a) and under simultaneous pulsed 145 eV Kr^+ ion action 0.5 s in duration and an ion current density of 0.6 μA cm^{-2} (b). The arrows indicate the times of ion pulsed action.

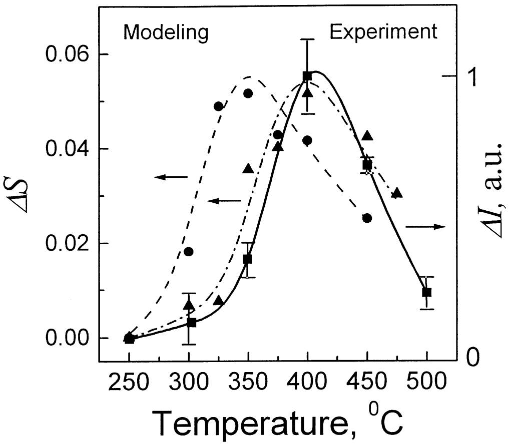

Fig. 2. Temperature dependence of ion beam induced RHEED intensity enhancement ΔI (■) and calculated value of enhancement ΔS at simulation parameters $E_1 = 1.1$ eV (●) and $E_1 = 1.2$ eV (▲).

meant that the Bragg diffraction conditions on the Si(111) surface were not disturbed by the ion beam action.

The lifetime of ion beam induced transformation providing surface smoothness during Si MBE is about one period of RHEED oscillations. This means that the deposition of one biatomic layer after pulsed ion beam irradiation seems to restore the surface to its original condition. The sequential pulsed ion beam actions on each growing layer, at a fixed degree of its filling $\theta = 0.8$, have shown the lasting RHEED intensity enhancement. The value of intensity enhancement ΔI was found to decrease slowly with an increase of number of deposited biatomic layers (Fig. 3b). It might be well to point out that the average RHEED intensity level slightly increased after pulsed ion beam irradiation. Keeping in mind the (7 × 7) virgin reconstruction of Si(111) surface before Si MBE, by analyzing the RHEED patterns we studied the superstructure phase transitions induced by pulsed ion beam in the temperature range from 350 to 500°C. The (7 × 7) virgin reconstruction of Si(111) is known to transform to a mixture of (3 × 3), (5 × 5), (7 × 7) and others after about one monolayer deposition during Si MBE on Si(111) [10]. The RHEED patterns were taken with a camera after interruption of Si MBE at $\theta = 0.8$. The interruption was made with a shutter. Then the electron beam Si evaporator was switched off to open the shutter for the pulsed ion beam irradiation of the Si wafer. It took ca 1 min to switch off the electron evaporator. Following opening of the shutter, the RHEED pattern was taken again just before and after ion beam action.

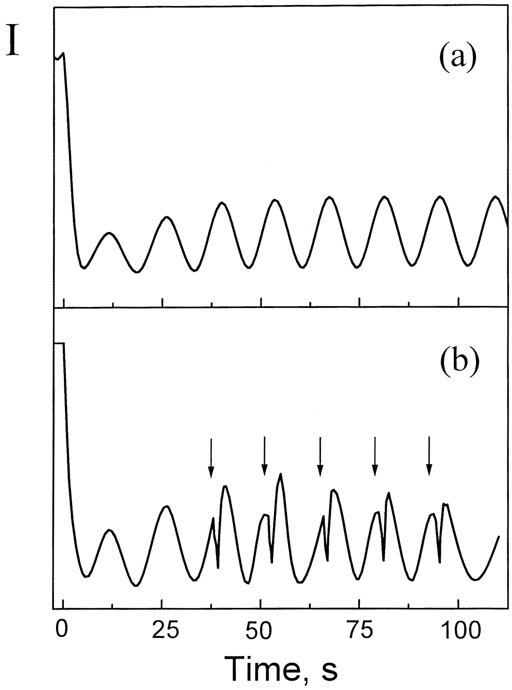

Fig. 3. RHEED intensity oscillations during Si epitaxial growth (a) and at multi-pulsed ion beam action on each growing bilayer at a fixed coverage of $\theta = 0.8$ (b). The substrate temperature is 400°C.

The characteristic time of the (7 × 7) superstructure recovery at a substrate temperature of ≤500°C is rather more than the operation time (ca 1 min) taken to get the RHEED pattern. According to Ref. [11], the mean domain sizes of (5 × 5) and (7 × 7) superstructures were invariable during the annealing time of a few hours at 500°C. Whereas at 600°C, the (7 × 7) domain size significantly changed within a few minutes. We controlled the recovery kinetics by comparison of RHEED patterns just after Si MBE interruption and before ion beam irradiation. In the temperature range studied these two patterns were the same for each substrate temperature.

We found an increase in the (7 × 7) reconstruction area $\delta_{7\times7}$ after pulsed low-energy ion beam irradiation (dashed line, Fig. 4). As the substrate temperature increases, the addition in the (7 × 7) reconstruction area $\Delta\delta_{7\times7}$ induced by the ion beam action was found to expand, and reached a maximum at 400°C (see inset in Fig. 4). Above this temperature the (7 × 7) reconstruction area tended to the value of common Si MBE without ion beam irradiation.

4. Growth model

The Si MBE under pulsed low-energy ion irradiation was investigated using Monte Carlo (MC) simulation. We used as a basis of our theoretical consideration the model of crystal growth on (111) surfaces of group IV semiconductors [7,8]. This model treats the crystal substrate as a diamond

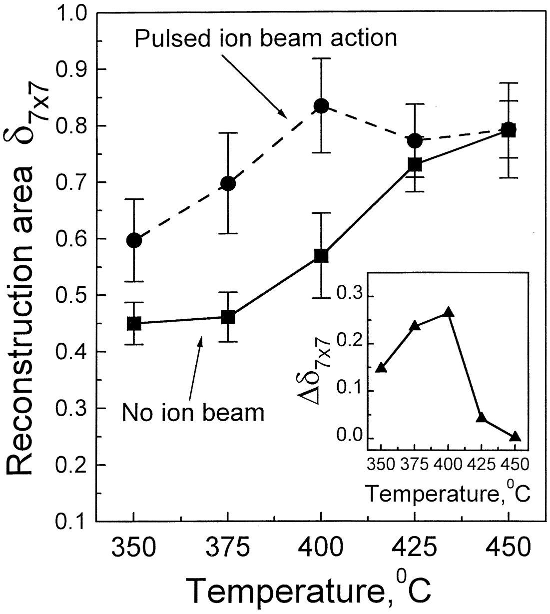

Fig. 4. Temperature dependence of the (7 × 7) reconstruction area $\delta_{7\times7}$ ca 1 min after interruption of Si MBE growth (■) and immediately after simultaneous pulsed ion beam action (●). Inset, the part of (7 × 7) reconstruction area $\Delta\delta_{7\times7}$ induced by ion beam irradiation (▲).

lattice in which volume vacancies and overhangs are forbidden. The thermal activity is restricted to surface atoms through nearest-neighbor hopping. Two kinetic processes are included in the growth description: the deposition of atoms from molecular beam; and the diffusion of adatoms. Growth is initiated by random deposition of atoms onto the surface. Surface migration is modeled by an isotropic nearest-neighbor hopping rate with an Arrhenius form:

$$\nu(E, T) = \nu_0 \exp\left(\frac{-E}{k_B T}\right), \qquad (1)$$

where ν_0 is the vibration frequency of the surface atoms, k_B is Boltzmann's constant, T is the substrate temperature, E is the activation energy of surface diffusion, which depends only upon nearest-neighbor environment of surface atoms. The activation energy is given by:

$$E = nE_1 + mE_2, \qquad (2)$$

where E_1 is the nearest-neighbor binding energy, E_2 is the next nearest-neighbor binding energy, n is the number of nearest-neighbors ($n \leq 3$) and m is the number of next nearest-neighbors in plane parallel to substrate ($m \leq 6$).

The diamond structure of Si(111) means that the stacking sequence consists of two alternative types of layers. Adatoms on one type of layer are bound by one bond to the surface ($n = 1$) while adatoms on the other layer type are bound by three bonds ($n = 3$). The important peculiarity of homoepitaxy on Si(111) is that the initial (7 × 7) reconstruction transforms to a mixture of (7 × 7) and (5 × 5) superstructure domains. As a result, the mobility of adatoms becomes lower than that on the virgin surface. To include surface reconstruction in the growth model, the diffusion activation energy was modified as follows [8]:

$$E = nE_1 + mE_2 + kE_3. \qquad (3)$$

Here kE_3 is the contribution from surface reconstruction, k is an integer (from 1 to 7) depending on the number of atoms in the layer below. The initial carefully prepared Si(111) surface with the (7 × 7) superstructure is assumed to have $E_3 = 0$. During the growth of the first biatomic layer there is a gradual increase in kE_3 due to the change in the surface reconstruction, which has a higher diffusion activation energy than that of the virgin surface [10].

The surface morphology during MC simulation is monitored by calculating the step density S. This quantity is proportional to the number of atoms along the perimeter of islands and vacancy clusters. It has been shown that $1 - S$ is proportional to specular RHEED intensity profiles in a variety of circumstances [8]. In the present study S is given by the following expression:

$$S = \frac{1}{4M} \sum_{i=1}^{\sqrt{M}} \sum_{j=1}^{\sqrt{M}} \left[|h_{i,j} - h_{i+1,j}| + |h_{i,j} - h_{i,j+1}| \right], \qquad (4)$$

where M is the number of the surface lattice sites, $h_{i,j}$ is the height of the surface at point (i, j).

The results of molecular dynamic (MD) simulation of low-energy ion interactions with Si(111) surface [12] are used as input for our MC simulation to take into account with the modifications of the surface morphology with ion beam action. According to the MD results, ion impact on a Si(111) surface produces one vacancy cluster. The average number of vacancies in the cluster is 16, one atom is sputtered and 15 atoms are excited in adatom positions. Since our experiments have established that pulsed ion action leads to increasing of (7×7) reconstruction area (Fig. 4), we have developed the growth model which includes surface reconstruction at ion irradiation. It is supposed that the ion beam action induced $(5\times5)\Rightarrow(7\times7)$ phase transition allows a decrease in the activation energy of adatom diffusion and improves the surface smoothness at Si MBE. To simplify the problem, we assume that:

1. experimental ion flux is enough to reconstruct whole surface (it corresponds to $E_3=0$);
2. the pulsed ion action is the process by which instant adding of surface modifications from each ion impact happens; and
3. the ion induced (7×7) reconstruction transforms to other surface phase after deposition of the one bilayer.

5. Results of modeling

The MC modeling was performed on a 147×147 lattice whose sites corresponded to regular atom positions in the crystal Si(111) surface. The growth of Si(111) is simulated in the temperature range of 250–550°C at a deposition rate of silicon 0.1 bilayer s^{-1}. The ion dose in a single pulse was taken as $10^{12}\,\mathrm{cm}^{-2}$. The following parameters were used in the simulation: $v_0=10^{13}\,\mathrm{s}^{-1}$, $E_1=1.1$ (1.2) eV, $E_2=0.2$ eV, $E_3=0.02$ eV. The periodic boundary conditions were employed at the lattice edges.

It was found that MC modeling results fit the main experimental data of RHEED intensity oscillation enhancement by pulsed low-energy ion beam action for different surface coverage and substrate temperatures. The simulation shows that the surface step density decreases after pulsed ion action. This effect was significant at surface coverage in range of $0.6<\theta<0.9$. To compare modeling with the experimental data we calculated the time and temperature dependent function $(1-S)$, which is similar to experimental RHEED oscillations [8]. Here S is given by Eq. (4). The minimum of the step density S or maximum of the $(1-S)$ was found at $\theta=0.8$ (Fig. 5a). There was practically no effect in the initial stages of the surface filling (Fig. 5b). The difference in values of $(1-S)$ between the ion-bombarded (—, Fig. 5a) and common growth (---, Fig. 5a) surfaces equals the oscillation enhancement ΔS. It was revealed, that this value depends on the temperature like a RHEED intensity oscillation enhancement ΔI in experiments (Fig. 2, for $\theta=0.8$). The peak of temperature dependence of ΔS (--- in Fig. 2) is defined by only one model parameter E_1. The modeling results at $E_1=1.2$ eV is in good agreement with the experimental temperature dependence. The reduction of E_1 shifts peaks of simulated dependence to lower temperature ranges.

The multi-pulse ion action is simulated as subsequent pulse ion actions on each growing layer at a fixed degree of its filling $\theta=0.8$. The modeling has shown that the minimal step density reached on the growth of the first few biatomic layers. As

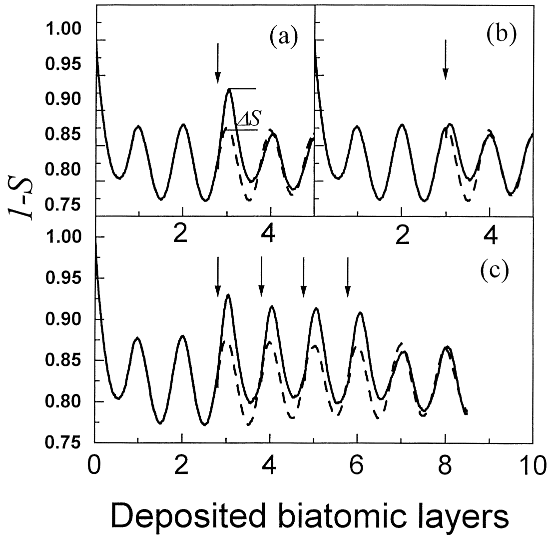

Fig. 5. Simulated step density evolution during Si(111) epitaxial growth (rate of 0.1 bilayer s^{-1}, $T=400$°C) with single (a and b) and multi (c) pulsed ion beam irradiation. Surface coverage $\theta=0.8$ (a and c) and $\theta=1$ (b). Simulation parameters: $E_1=1.2$; $E_2=0.2$; and $E_3=0.02$ eV.

further atomic layers are deposited, the effect of the ion beam becomes weaker. The calculated value of intensity enhancement ΔS under multi-pulse ion beam action was damping with an increase of deposited bilayers (Fig. 5c), as for the experimental data (Fig. 3b).

Step density evolution during MBE has been calculated under single-pulse ion beam action on a surface at $\theta = 0.8$ with a different number of deposited layers. In every computational experiment MBE growth started from the virgin Si(111) surface it was found that ΔS slightly decreased as the number of deposited layers increased (Fig. 6). These results show the reason for the damping of the ion beam induced surface smoothness improvement at multi-pulse irradiation with fixed phase (coverage). The reason is the surface roughness build-up for thicker deposited layers.

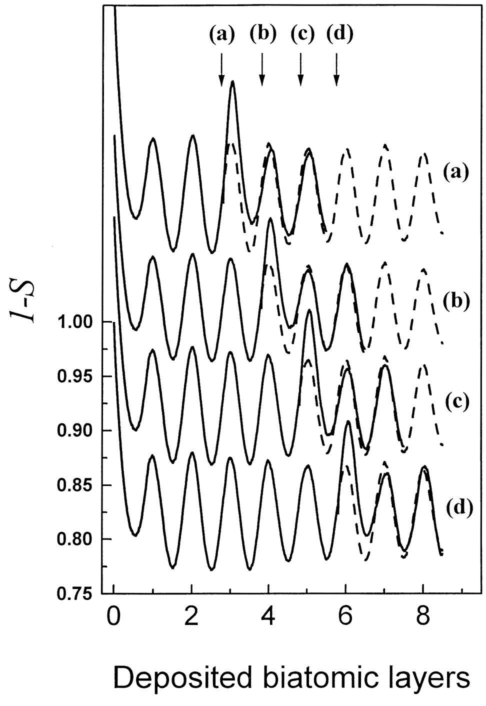

Fig. 6. Simulated step density evolution during Si MBE under single-pulse ion beam action ($\theta = 0.8$) on a surface with different number of deposited bilayers: (a) 2.8; (b) 3.8; (c) 4.8; (d) 5.8 bilayers.

6. Discussion

Finally there is a similarity between the results of works on synchronization of nucleation [3,13,14] and low-energy ion-pulse action from the position of improving of the surface smoothness by the external energy source action. Synchronization of nucleation was firstly reported by Markov et al. [3] to improve the homoepitaxial growth of Si on Si(111) and Ge on Ge(111). They increased the substrate temperature at each minimum or increased the rate of molecular beam (approximately by a factor of 4) at each maximum RHEED amplitude oscillation momentarily and kept these conditions for a quarter of the period of layer growth. The RHEED oscillations minima correspond to maxima in the step density and by temporarily increasing the surface diffusivity with heating, the layer-by-layer growth was promoted. It can be formulated that the temperature modulation synchronizes the nucleation of each layer by giving a large supersaturation via a reduced temperature at the onset of growth of each layer. Later Larsson et al. [13,14] using RHEED intensity oscillations investigated the nucleation and island growth for MBE of Si on Si(111) and the heteroepitaxial growth of $Si_{1-x}Ge_x$ on Si(111) during intermittent radiant heating.

The higher molecular beam rate increases supersaturation during growth of the first part of the growing layer to stimulate islands nucleation. This was shown to lead [3] to longer lasting RHEED oscillations (i.e. better growth).

RHEED intensity enhancement by pulsed ion beam under Si/Si(111) homoepitaxy gives an indication of a decrease in the surface density of electron scattering centers which are the Si islands and depleted zones. A number of elementary atomic processes accompanying ion-stimulating growth may provide a contribution to the observed improvement of the surface smoothness:

1. sputtering of Si atoms which is similar to the rate reduction of the molecular beam;
2. surface heating by ion energy deposition and an increase in adatom diffusivity;
3. the influence of the beam impurity as a surfactant on Si/Si(111) homoepitaxy;
4. modification of the growth kinetics in

adatom/vacancy-mediated epitaxy under ion bombardment (for example, pulsed ion beam would lead to small Si islands as lower temperature/higher rate does); and
5. surface phase transitions induced by ion action.

Taking the sputtering coefficient to be equal to 1, we find that the number of sputtered atoms (equal to the irradiation dose) is ca. 1% of the number of atoms deposited from the molecular beam over the time of ion irradiation. This rate reduction is too low to induce a noticeable modification in the growth kinetics. The sputtering effect was shown to be important when the ion flux matched the molecular beam flux [15,16].

Taking a look at individual ion–solid interaction, one may estimate that the characteristic time of energy dissipation equals 5–10 ps [17]. The adatom diffusion length over this time does not exceed 0.03 nm. This is much smaller than the average size of the surface thermal spike (~ 10 nm) induced by a single ion strike and the mean spacing between ion's impacts (~ 10 nm) at doses used experimentally. The collision events are separated by ca. 1 s at a current density of 0.6 μA cm^{-2}. So the each ion–solid interaction occurs on a surface cooled down to the initial substrate temperature.

Taking into account just the adatom and vacancy clusters generation by pulsed ion action, we simulated the growth with a MC code. The results revealed that there is no surface smoothness improvement for all the current densities, deposition rates and substrate temperatures used in our experiments. The ion current and irradiation doses are apparently too low to influence the surface morphology with adatom/vacancy generation.

Recently the influence of some impurities as surfactants on Si homoepitaxy was studied. The elements of group III (In, Ga) and IV (Sn, Pb) were found to increase diffusion length, while hydrogen and the elements of group V (As, Sb, Bi) and VI (Te) reduced diffusion length [18]. The inert gases were not found to influence Si homoepitaxy. The superstructure phase transition observed in this paper is suggested to be induced by energetic ion bombardment.

Hence the first four processes mentioned above hardly contribute to ion beam induced surface smoothness improvement. Multi-collision phenomena and ion beam sputtering could not be simply described with a thermal or rate effect. This means that microscopic phenomena at low-energy ion irradiation are different from those caused by periodically altering the substrate temperature and rate.

The growth simulation results are in good agreement with the experimental data if surface reconstruction by pulsed ion beam action was taken into account as shown in Section 4. Fig. 7a shows the simulated surface morphology after deposition of 2.8 bilayer at $T = 400°$C with a deposition rate of 0.1 bilayers s^{-1}. The higher levels of the Si atom position are marked with lighter gray shades, and lighter zones in the figure correspond to islands and darker zones are depressions in the surface layer. Fig. 7b shows the surface image at an ion beam action with dose of 10^{12} cm^{-2}. Nearly the same surface morphology can be recognized in the both images due to the low irradiation dose and the small density of defects induced by ion beam. As was shown by us ion beam pulsed action leads to surface phase transition from the (5×5) metastable phase to the (7×7) phase. The activation energy of adatom migration is smaller for (7×7) reconstruction as compared with a mixture of superstructures [10]. That is why the Si adatoms deposited from the molecular beam to Si(111) surface, reconstructed by pulsed ion beam, were able to fill the vacancy depressions, and provide smaller density of islands (Fig. 7d) as compared with common MBE (Fig. 7c). As a result of this, the simulated surface step density decreases (Fig. 5b) and the specular RHEED intensity increases (Fig. 1b) after ion beam pulsed action during Si homoepitaxy.

Now we focus on the temperature dependence of ion beam induced surface smoothness. Silicon homoepitaxy proceeds in nucleation, growth and coalescence of two-dimensional islands. Nucleation of new islands and growth of existing islands are competing processes. The contribution of both processes is determined by adatom diffusion, on the one hand, and the number of atoms and the energy to form stable nuclei on the other hand. Around existing islands adatoms diffusion to and incorporation in the islands reduce the adatom density. If we take the mean distance

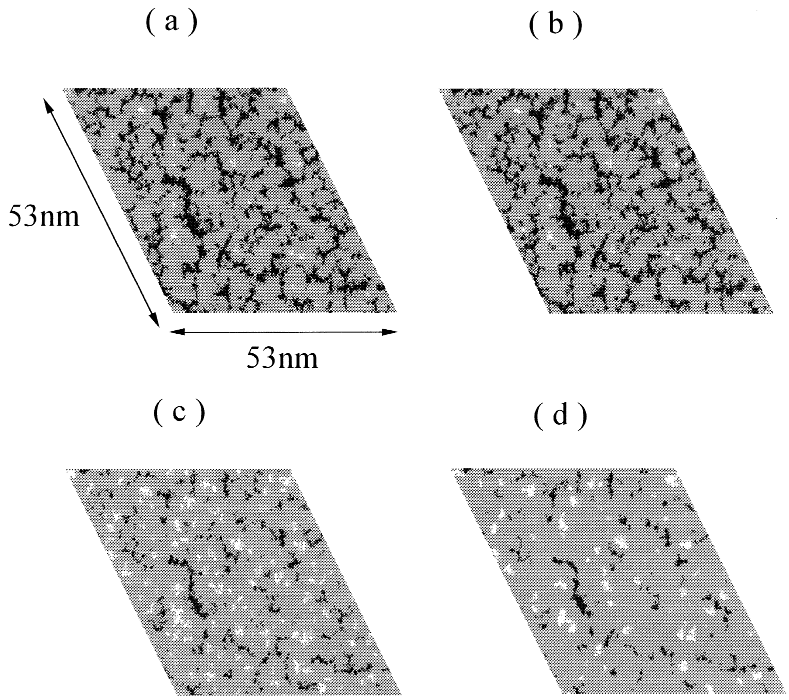

Fig. 7. Simulated surface images: (1) before (a) and after (b) pulsed ion beam modification at surface coverage $\theta=0.8$; (2) after subsequent growth on (a) and (b) surfaces up to $\theta=1$; (c) no ion beam; (d) post-ion beam modification growth. The deposition rate was 0.1 bilayer s^{-1}, the substrate temperature was 400°C, the ion dose was 10^{12} cm^2. The size of the surface cell was 53 nm × 53 nm. Higher levels are marked with lighter gray shades in the images.

between these islands as a characteristic length for the adatom diffusion, this length L is related to the island density N by $L=N^{-1/2}$.

In a low temperature range the diffusivity decreases and the island density increases. The new nuclei could be formed over existing islands long before the previous layer is completed. In this case the diffusion length is mostly controlled by the incorporation of atoms in the steps rather then the surface superstructure. So, even the surface reconstruction with ion beam action leads to an increasing in adatom mobility and the step density is not reduced.

As the substrate temperature increases, the diffusivity grows. L increases and correspondingly the island density decrease. Ion beam assisted (5 × 5) to (7 × 7) phase transition enhances adatom diffusion and, additionally, contributes to a smoother surface. The (7 × 7) reconstruction area shows increases as the substrate temperature rises (Fig. 4). That is why within a high temperature limit the contribution from the ion beam induced (7 × 7) reconstruction practically disappears.

We may explain the dependence of the ion beam effect on the number of layers grown by the kinetic build-up of roughness through deposition on a flat surface. A gradual build-up of roughness is induced as the thickness of epitaxial layer increases [3].

7. Conclusion

We have studied the initial stages of low-temperature (200–600°C) Si/Si(111) molecular-beam epitaxy under the action of pulsed (0.25–1 s) low-energy (~100 eV) ion beam. The ion beam induced surface smoothness improvement was found to depend strongly on the surface coverage and the substrate temperature. The ion beam influence is naturally highest for systems closest to the surface coverage $\theta=0.8$, and at substrate temperature of ca 400°C. During Si/Si(111) MBE there is known to be a mixture of surface superstructures. We have found that ion beam irradiation of short duration leads to an increase in the (7×7) reconstruction area. This area grows as the temperature of the substrate increases and reaches a maximum ca 400°C. For higher temperatures the contribution of ion beam induced (7×7) reconstruction is reduced and tends to the values of common Si MBE without ion bombardment. We present a simulation model of Si/Si(111) MBE under pulsed low-energy ion beam action, which induces (5×5) to (7×7) phase transition. In view of the fact that the activation energy of Si atom surface diffusion increases under transition from a mixture of superstructures to mostly single (7×7) reconstruction, the pulsed ion beam irradiation offers the lower activation energy for adatom diffusion. Under this assumption the modeling results fit to experimental data at different surface coverages for different substrate temperatures for both single and multi-pulsed ion beam actions.

The technique developed and phenomena observed offer a new way of MBE with synchronization of structure transformations by pulsed low-energy ion beam action. The advantages of this technique are the low epitaxy temperature and phase (coverage) sensitive surface smoothness improvement.

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