Growth mechanisms of Si and Ge epitaxial films on the dimer reconstructed Si{100} surface via molecular dynamics

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Microscopic and macroscopic growth mechanisms of thin epitaxial films due to Si and Ge deposition on the Si{100}-(2×1) surface are studied via molecular dynamics using Tersoff's many-body potential. The dimer openings on the reconstructed surface following the Si or Ge deposition are either due to a diffusing adatom induced mechanism or due to a direct insertion of the incoming adatoms into the epitaxial positions. Two distinct layer by layer growth modes of macroscopic epitaxial films are observed; (a) the mode in which the domains of good or bad epitaxial growths remain roughly in the same area of the interface throughout its entire thickness, and (b) the mode in which reconstructions on the buried interfaces can be relieved by long time equilibrations, i.e., the epitaxially deposited film can heal its inner layers during equilibrations. The qualities of the final macroscopic films in these two cases are found to be distinctively different.

I. INTRODUCTION

The growth of high quality epitaxial semiconductor thin films by molecular-beam epitaxy (MBE) is a subject of intense theoretical and experimental investigation due to its direct relevance to the advances in the semiconductor technology. The availability of realistic many-body potentials for silicon,[1] carbon,[2] and germanium[3] have made it possible to study the epitaxial growth of these semiconductors by using molecular dynamics (MD) simulations. In MD simulations the gas phase atoms of the semiconductor materials are randomly deposited on a substrate maintained at a constant temperature. The nonequilibrium dynamics of the whole system is evolved by integrating classical equations of motions in finite short steps in time. One of the main problems encountered in any simulations of the epitaxial growth is the correlation of MD simulation rates, which are typically of the order of few monolayer (ML)/nanosecond,[4] to the experimental growth rates which are of the order of 0.1 ML/min.[5] This is overcome by deposition of the incoming atoms at a much faster rate, and the equilibration of the full system with the hope that all the rare event processes such as diffusion, evaporation, and migration of the deposited atoms do take place during the equilibration. In the simulation results reported in this work, after each deposition of about 1.5 ML of material, we have followed the motion of all the deposited and the substrate atoms typically for about 0.5-1 ns so that the microscopic motion of all the deposited material can be understood on a layer by layer basis. In the earlier work of using MD simulations to study the epitaxial growth,[6,7] efforts were focused mainly on achieving the deposition of few monolayer thick epitaxial films, thus the macroscopic features of the deposited film were emphasized. In other studies of the microscopic mechanism of the earlier stages of the epitaxial films[8] using the Brenner–Garrison potential,[9] the dimer opening mechanism of the dimer-reconstructed Si{100}-(2×1) surface was studied in detail, however, the macroscopic deposition of few ML thick epitaxial layer was never achieved. Recently, using Tersoff's many-body potential for Si–Si interactions[10] we have reported a microscopic mechanism of the initial stages of the epitaxial growth of Si on the Si{100}-(2×1) surface, and have also successfully grown about 4 ML of the Si epitaxial film.[4] Since Tersoff's potential for multicomponent Si, Ge, and C systems is already reported in the literature,[11] it is straightforward for us to test the quality of these potentials for the pseudomorphic growth. As the lattice constant of Ge is about 4% larger than that of Si, a Ge thin film epitaxially grown on the Si{100} substrate has a uniaxial strain perpendicular to the {100} crystal face. It has been observed experimentally[12] and also shown in some theoretical studies[13] that this strain can readily effect the electronic and optical properties of the material. Si/Ge interfaces are also interesting from a technological point of view because they offer the possibility of constructing heterojunctions which can be integrated directly with the existing Si circuits. In this work, we present results on our recent MD simulation of the epitaxial growth of Si and Ge thin films on the dimer reconstructed Si{100}-(2×1) surface using Tersoff's potential for a multicomponent Si and Ge system. The microscopic nature of dimer openings due to the deposition of Si and Ge atoms is broadly classified into; (a) diffusing adatom induced dimer openings,[4] and (b) direct insertion of incoming adatom into the epitaxial position. The relative significance of these two mechanisms and their effect on the macroscopic growth modes of the epitaxial films are discussed. The diffusing adatom induced dimer opening mechanism is responsible for the anisotropic nature of the epitaxial growth in the initial stages observed in both Si and Ge deposition. It is also noted that the macroscopic nature of the growth of Ge/Si{100} is quite different from that of Si/Si{100}. In Sec. II, we briefly discuss the simulation system, and the interaction potential employed in this work. Section III A

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describes microscopic mechanisms of dimer openings due to Si and Ge deposition on Si{100}-(2×1) surface. Section III B reports in brief the microscopic and macroscopic characteristics of the growth of Si/Si{100}, readers are referred elsewhere[4] for a detailed description. In Sec. III C we describe the growth of few ML thick Ge/Si{100} thin film, and last in Sec. IV we comment upon the microscopic and macroscopic growth characteristics of the Ge and Si epitaxial films.

II. SIMULATION SYSTEM AND THE INTERACTION POTENTIAL

Our MD simulation consisted of maintaining ten layers of 32 atoms/layer at a constant temperature by fixing the bottom most layer, and considering the atoms in the next four layers as forming a stochastic region. The thermal equilibration of the whole system was maintained by using friction forces[14] only in the stochastic region. This means that the top five layers of the system were considered as the interaction region, in which the equations of motion contained forces due only to the many-body potential function. This makes the dissipation of excess energy into the lower layers of the stochastic region rather slow, but the dynamics in the interaction region is more accurate and therefore is a better representative of the dynamic behavior of the interaction potential. The initially reconstructed surface was defect free and was equilibrated at the desired temperature. This top layer had initially 16 dimers which were arranged in rows, and the periodic boundary conditions were employed along the surface plane. This structure has been shown in our previous simulation of the deposition of Si/Si{100},[4] and has also been observed in the direct scanning tunneling microscopy (STM) studies.[15] Si and Ge atoms were deposited at a rate of 1 atom /2–3 ps, a sufficiently slow rate to equilibrate the deposited atom before the arrival of the next. After the deposition of each 1.5 ML (for Si{100} surface 1 ML $= 6.782\times10^{14}/\text{cm}^2$), the full system was equilibrated 0.5–1 ns to study the dynamic behavior of the deposited and the substrate atoms on a microscopic level.

The interaction potential used in these simulations is Tersoff's many-body potential for Si and Ge.[11] In a previous study of the MBE growth of Si/Si{100} system, we have used this potential and have found that for the dimer reconstructed {100} surface it not only gives reasonable energetics of the dimer reconstruction (1.45 eV/dimer) but is also suitable for the simulations of the epitaxial growth. It is noted that in Tersoff's potential the heteroatomic interaction between Si and Ge atoms is introduced simply by a single additional parameter. The rest of all the other parameters are either the arithmetic or the geometric means of the parameters for the isolated Si and Ge atoms, and the functional form of the potential for a multicomponent system remains same as that of the previous single component case.

III. RESULTS AND DISCUSSION

A comprehensive picture of the initial stages of the growth of thin epitaxial films on the Si{100}-(2×1) surface includes not only the atomic level details of the individual dimer openings (an essential step for the initiation of the epitaxial growth), but also the macroscopic view of the layer by layer deposition process. We first present the microscopic mechanism of individual dimer openings due to Si and Ge adatom deposition, and then describe the layer by layer growth modes of few ML thick Si and Ge epitaxial films.

A. Microscopic mechanisms of dimer openings in the initial stages of the epitaxial growth

The microscopic mechanisms of stable dimer openings (those dimers that remain open for the entire duration of simulation) are basically of two types. First is the diffusing adatom induced mechanism, the typical examples of which are shown in Figs. 1(a) and 1(b). As observed and explained in detail in our previous work,[4,8] the adatoms move as shown by the arrows in Fig. 1(a) during the equilibration period (0.5–1.0 ns). First, both the dangling bonds of an isolated dimer are saturated with two adatoms. A third adatom diffuses over a period of hundreds of picoseconds, to move closer to the dimer, and pushes the adatom on the dangling bond into the epitaxial position. The diffusing adatom itself then occupies the vacant dangling bond of the open dimer. The three adatoms finally occupy the epitaxial positions, whereas the dimer atoms have relaxed back to their bulk positions. Another observed mechanism of the diffus-

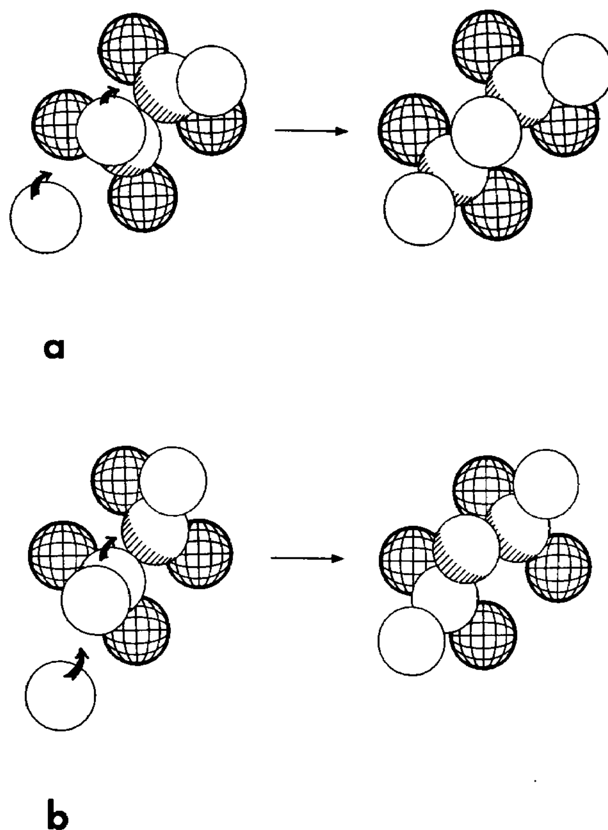

FIG. 1. (a) Diffusing adatom induced mechanisms of dimer openings. The inner layer Si atoms are hatched circles, the top dimerized layer are the shaded circles, and the Si or Ge adatoms are shown as open circles. The curly arrows indicate roughly the positions to which adatoms will move in the next 0.5–1 ns of equilibration. Open dimers and epitaxially placed adatoms are shown as the final product. (b) Same as (a) except that the mechanism is that of the formation of a defect (see the text).

ing adatom induced dimer opening is shown in Fig. 1(b). Instead of pushing the adatom on the dangling bond into the epitaxial position, in this case, the diffusing adatom can move underneath the adatom on the dangling bond and push the dimer atom into the epitaxial position. In this case, the diffusing adatom has moved into the top substrate layer whereas the substrate dimer atom has moved up into the epitaxial layer. The end products in the homoepitaxy of Si/Si or Ge/Ge, as shown in Figs. 1(a) and 1(b) are the same. However, in case of the heteroepitaxy of Ge/Si this will cause the formation of a defect at the interface.

In the second distinct mechanism of surface dimer openings the atoms in a surface dimer are constantly in motion about their equilibrium positions with amplitudes fixed by the temperature of the substrate. During these motions the surface dimers would spontaneously open sufficiently far from their equilibrium separation so that an incoming adatom is directly inserted into the available epitaxial position and stabilize the opening. As shown in Figs. 2(a)–2(d), we found that the direct insertion of the adatom into epitaxial positions can occur on a bare dimer, on a dimer with one of the dangling bonds occupied, and also on a dimer with both of its dangling bonds occupied. Most of such direct insertion mechanisms occurred during the deposition process, i.e., the surface was relatively clean. The number of such occurrences increased with an increase in the temperature of the substrate. Above room temperature (800 and 1200 K) and during the equilibration period, it was also noticed that occasionally a spontaneously opened bare dimer on a relatively clean surface would remain open for hundreds of picoseconds until being stabilized by the direct insertion mechanism. At higher temperatures (1200 K as compared to 800 K for the Tersoff Si potential) the direct insertion mechanism was the primary reaction mechanism of surface unreconstructions.

In a similar study[8] of the epitaxial growth using a different interaction potential,[9] the diffusing adatom motion mechanism was the main mechanism of stable dimer openings, but the total number of such observed openings during 0.5 ns equilibration period was comparatively smaller. Therefore, no macroscopic layer growth of few ML was achieved. In the same study some unstable open dimers due to the insertion of two or more adatoms were also observed. These unstable openings and the resultant structures are not observed in the present simulations. We believe that the higher surface stabilization energy of that potential[9] (2.1 eV/dimer) versus (1.45 eV/dimer) for the Tersoff's Si potential[10] and the shorter equilibration times of that simulation may have caused the observed differences.

B. Epitaxial growth of Si/Si{100}

Detailed results of the MD simulation of up to 4-ML thick Si thin film on Si{100} substrate are presented elsewhere.[4] Here we briefly summarize the main features of the results. We found that the unreconstruction of the (2×1)-Si{100} surface due to Si deposition at 800 K is mainly due to the diffusing adatom induced mechanism of dimer openings. A correlated diffusion induced openings of the neighboring dimers, in which the diffusing adatoms move perpendicular to the direction of the dimer rows on the original surface and open successive dimers, was observed. This mechanism was proposed for being responsible for the anisotropic nature of the epitaxially grown layers at low coverage as observed in

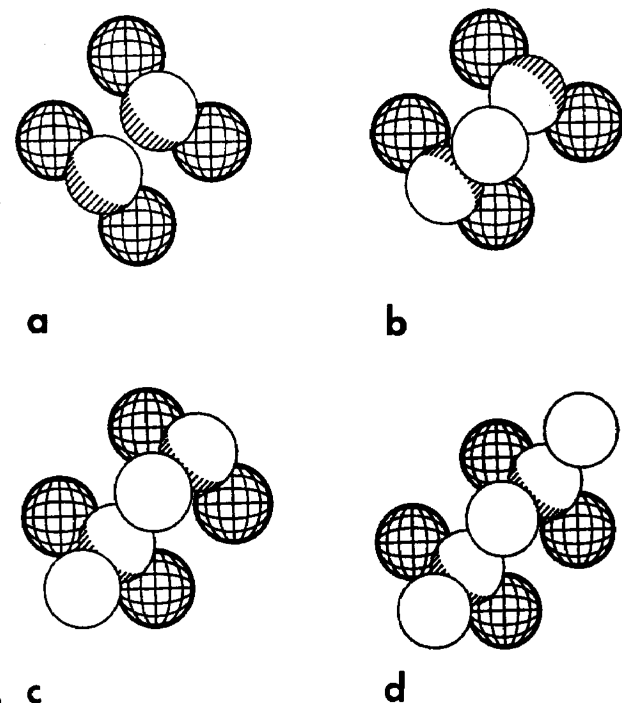

FIG. 2. (a) Inner layer Si atoms and a bare dimer. (b) direct insertion of the incoming adatom into epitaxial position (c) and (d) are same as (b) except that either one or both of the dangling bonds of the original dimer are occupied.

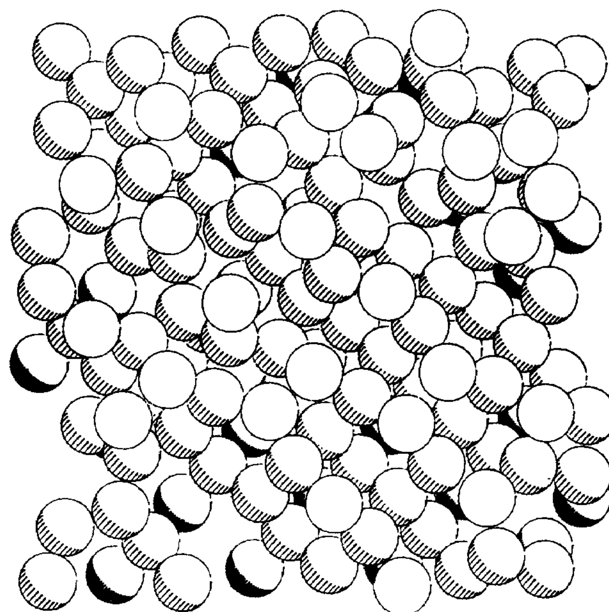

FIG. 3. Si{100} surface with a 4-ML thick epitaxial Si film. Atoms in the original dimerized layer are dark shaded circles, and the rest are the deposited Si atoms. Atoms in the first, second, and third epitaxial layers are light shaded circles, whereas the atoms in the topmost epitaxial layer are open circles.

recent STM studies.[16-18] The epitaxial growth of a 4-ML thick Si thin film was achieved. The study of the macroscopic nature of the growth mode revealed a layer by layer epitaxial formation, i.e., the top layer was constantly reconstructing and the next to the top layer was constantly unreconstructing. It was also noticed that the growth characteristics of the initially deposited epitaxial layers are continuously passed on to the later deposited layers. This means that the domains of good epitaxial growth in all first four deposited layers remain roughly in the same area of the substrate in which the dimer atoms had rearranged back to their bulk positions. For example, in Fig. 3 we show the final result of the epitaxial growth of up to 4 ML of the deposited material. This was obtained by three successive depositions of 1.5 ML, each of which followed by about ~ 1 ns equilibration. The lower right and the upper left portion of the figure show good epitaxial growth in all four layers. The upper right corner shows the amorphous region which also penetrates through all four layers.

C. Epitaxial growth of Ge/Si{100}

The simulation of the epitaxial growth of Ge layers on a fixed Si substrate at 800 and 1200 K was performed. The dimer openings on the reconstructed Si surface was mainly due to the direct insertion of the incoming Ge atoms into the epitaxial positions (Fig. 2). The number of such openings due to Ge atoms deposition increased by increasing the temperature of the substrate from 800 to 1200 K. At 800 K, however, as the substrate was equilibrated for ~ 1.0 ns after the deposition of 1.5 ML not even a single additional opening due to the diffusing adatom motion induced insertion was observed. A further deposition of another 1.5 ML and the subsequent equilibration of ~ 1 ns also did not open any additional dimers. So it was concluded that for the given potential at 800 K the reconstructed Si{100} surface does not show any appreciable dimer opening due to Ge adsorbate motion.

The simulation of Ge deposition on the (2×1) dimer reconstructed Si substrate maintained at 1200 K was also carried out. The insertion of incoming Ge atoms into the epitaxial positions to stabilize a spontaneously opened dimer was the main mechanism of surface unreconstruction during the deposition period. A couple of diffusing adatom induced dimer openings during the equilibration of the initially deposited 1.5 ML were also observed. In Fig. 4, we show the dynamic evolution of the first epitaxially deposited Ge layer as the full simulation of the deposition and equilibration of up to 4.5 ML Ge atoms is performed. Figure 4(a) is after the deposition of the first 1.5 ML of Ge atoms. Nine dimers on the fully reconstructed Si surface have opened during this deposition. Of these, six were due to the direct insertion mechanism (Fig. 2), and the remaining were due to the diffusion induced mechanism (Fig. 1). For clarity, only those Ge atoms which were at the level of the first epitaxial layer are shown. Figure 4(b) shows the Si substrate and the Ge layer of Fig. 4(a) equilibrated for about ~ 0.5 ns. A further opening of two more dimers due to the diffusion induced mechanism has occurred. At this stage of the simulation, i.e., after the deposition and equilibration of ~ 1.5 ML, we note

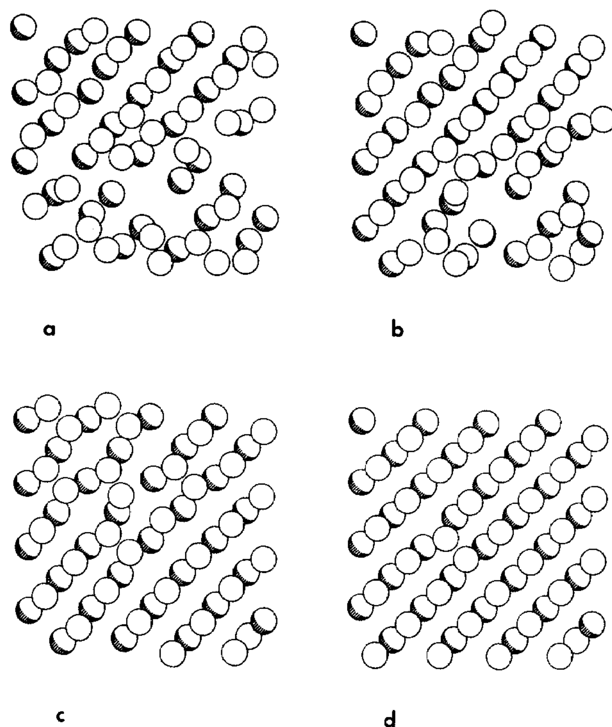

FIG. 4. Dynamics of the original Si{100}-(2×1) surface and the first Ge epitaxial layer. The shaded circles represent the surface dimer atoms, and the open circles are the deposited Ge atoms. (a) The surface after the deposition of 1.5 ML Ge atoms, of which only the atoms in the first epitaxial layer are shown. (b) The Ge/Si interface after the equilibration of ~ 0.5 ns. At this stage in simulation (~ 0.63 ns) about 0.7 ML of the original Si surface is unreconstructed and 0.7 ML of the deposited Ge atoms are in the epitaxial positions. (c) The Ge/Si interface after the deposition and equilibration of another 1.5 ML Ge atoms (~ 1.3 ns). All the dimers on the original Si surface are open and the first epitaxial Ge layer is complete. The upper left corner of this figure shows (2×2) dimer reconstructions in the deposited Ge layer. (d) Ge/Si interface after another deposition and equilibration of 1.5 ML Ge atoms. The earliest deposited Ge atoms on the interface have equilibrated for 2.2 ns. The (2×2) dimer reconstruction in the Ge epitaxial layer is almost relaxed. Only a single Ge dimer is left on the interface, which by now is buried under about 3.5 ML of Ge atoms.

that about 0.70 ML atoms of the originally reconstructed Si surface have been reordered back to their expected bulk positions, and about 0.70 ML of the deposited Ge atoms are in the epitaxial positions. The time evolution of the first epitaxial layer during the deposition and equilibration of the additional 3 ML of Ge atoms are shown in Figs. 4(c) and 4(d). In Fig. 4(c) the original Si surface and the first epitaxial Ge layer at about 1.3 ns in the simulation is shown. One notes that by now all the dimers in the fully reconstructed original Si surface in the beginning of the simulation have opened. However, in the upper left corner of the figure about one third of the first Ge epilayer has (2×2) dimer reconstructions. After the deposition and equilibration of additional 1.5 ML Ge atoms, the first epitaxial Ge layer and the original Si surface at about 2 ns are shown in Fig. 4(d). At this point in simulation, the originally reconstructed Si surface is fully unreconstructed and the first Ge epilayer at the Ge/Si interface, which is buried under about 3.5 ML of additional Ge atoms, has only one reconstructed dimer left. In contrast to the growth of Si/Si{100}, the unreconstruction of the origi-

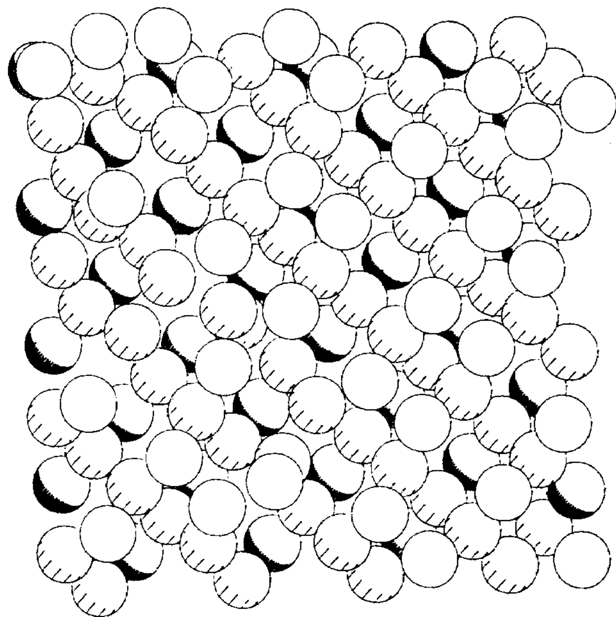

FIG. 5. Si{100} surface with 3-ML thick Ge epitaxial film. Si atoms in the original dimerized layer are dark shaded circles. Ge atoms in the first and the second epitaxial layers are light shaded circles, whereas the top most Ge layer atoms are open circles. The right half of the figure shows good epitaxial growth in all three layers, and the left of the center shows some amorphous region the origin of which can be traced back to the unopened Ge dimer at the Ge/Si interface [also see Fig. 4(d)].

nal Si surface and the first Ge epilayer at the Ge/Si interface which is buried under up to 3 ML of Ge atoms can occur during the nanoseconds time scale equilibration period. This means that the growth characteristics of the initially deposited Ge layers will change as the system is equilibrated because the buried reconstruction at the interface has a tendency to heal itself. In Fig. 5 we show the result of the epitaxial growth of up to 3-ML thick Ge epitaxial film on Si{100}. The full system at this point has about 4.5 ML of Ge atoms, and has been equilibrated for about 2 ns. For clarity the atoms at the level of the 4th, 5th, and 6th deposited layers are not shown. The surface shown in Fig. 5 has about four randomly placed dimers in the second Ge epilayer (upper left corner), and a good epitaxial growth of up to 3 ML in the right half. This shows that the good epitaxial growth in the deposited film is occurring first in the region where the dimers of the original Si surface and the first Ge epilayer had relaxed quickly to their bulk positions. In the left half of the Fig. 5, the epitaxial growth is not as good because there still are few unopened dimers in the underneath layers. However, from the dynamics of the first Ge epitaxial layer, as shown in Figs. 4(c) and 4(d), it is clear that left half of the deposited film may also heal completely if we deposit more Ge atoms and/or equilibrate for still longer times.

IV. COMMENTS

To summarize the inferences drawn from these simulations we first review the microscopic mechanisms of surface unreconstructions during the initial stages, and then comment upon the macroscopic features of the growth modes of Si and Ge epitaxial films. It is found that the openings of the dimers on Si{100}-(2×1) surface occur through two distinct mechanisms, (a) the diffusing adatom induced bumping of the adatom on the dangling bond into the dimer, and (b) direct insertion of the incoming adatoms into epitaxial positions. The former is the primary mechanism of unreconstruction during the equilibration process while the latter occurs mainly during the deposition process. Number of both types of such occurrences increase by increasing the temperature of the substrate. The diffusing adatom induced dimer opening [Fig. 1(b)] can also sometimes cause interlayer mixing across the growing interface. The growth of Si/Si{100} thin film, presented in detail elsewhere,[4] revealed a novel mechanism of correlated adatom motion induced dimer openings which is more favored in a direction perpendicular to the direction of the dimer rows on the original reconstructed surface. This mechanism may be responsible for the anisotropic nature of the epitaxially grown layers as observed in some recent STM studies.[16–19] In some recent work[18,19] it has also been pointed out that the systems that grow epitaxially, but in which there is a lateral growth anisotropy, will grow with a smaller interface width than the system in which the growth is isotropic. Technologically this is important because the anisotropic growth will favor a smoother interface as compared to the isotropic growth under the similar conditions. The dimer opening of the Si{100} surface due to Ge deposition was mainly through the direct insertion mechanism, however, few correlated adatom motion induced dimer openings were also observed. It is found that the Ge deposition completely relieves the reconstruction on the Si{100}-(2×1) surface at a higher temperature (1200 K) as compared to the unreconstruction due to Si deposition at 800 K. This is not in agreement with the experimental evidences in which the Ge deposition even at room temperature does relieve the reconstruction on the Si{100}-(2×1) surface.[5] We explain this disagreement in two ways. First, we note that Tersoff's potential used in these simulations,[11] fit to accurately produce bulk and surface elastic properties, does not give the correct melting temperature. Second,the predominant mechanism at the lower temperature, i.e., the diffusing adatom induced dimer openings during the equilibration period, may take much longer to occur for Ge atoms than for the Si atoms. The time scales of these longer duration processes for Ge deposition may not be feasible in the present simulations. Therefore, rather than concentrating on the exact temperature behavior we have concentrated on the detailed mechanism of many observed processes and the relative energetics of them.

Next, we compare mechanisms of the two macroscopic growth modes as observed in the simulation of Si and Ge epitaxial films deposited on the Si{100}-(2×1) surface. In the first case, the deposition of Si on Si{100} surface follows a layer by layer growth mode observed also in the Rutherford back scattering experiments.[5] It was noted that the top epitaxial layer is always reconstructing where as the next to the top layer is relaxing back to the bulk positions unreconstructing. Therefore, at any stage during the simulation, the unopened dimers in the area of good epitaxial growth mostly occur under 1-ML thick epitaxial film. However, in the re-

gions of amorphous growth, i.e., the region where dimers on the original (2×1) reconstructed surface did not relax to their bulk positions, the reconstruction could remain stable under as many as the full thickness (4–5 ML) of the epitaxially grown film. In other words, the growth characteristics of the earlier deposited layers are continuously passed on to the later deposited layers, i.e., the initially amorphous region stayed amorphous for the entire duration of the simulation. The macroscopic growth mode in the second case as observed in these simulations is distinctively different. The growth of a thin (4 to 6 ML) Ge epitaxial film is also a two dimensional layer by layer mode. However, the unreconstruction on the Si–Ge interface buried under up to 3.5 ML Ge atoms occurs during the equilibration process. This means that the reconstructed Si and Ge layers, in the presence of 2–3 Ge overlayers, can be relaxed back to their bulk positions during long time equilibration. Therefore, as the layer by layer growth of the epitaxial film is followed, the initially deposited layers with some unopened dimers, and thus the resultant amorphous regions in the later deposited Ge overlayers, had tendency to heal themselves to the good epitaxial positions in the later stages. This is in marked contrast with the buried interface of the previous case where the dimer reconstruction on the interface and the resultant amorphous regions in the overlayers remain as they are throughout the entire duration of the simulation. Although we have clearly identified two modes of rearranging reconstructions during growth, it is unclear the precise factors that determine when one or the other is operative. It is premature to definitively ascribe rearrangement at the surface to Si/Si{100} growth and rearrangement at the buried interface to Ge/Si{100} growth, as the characteristics of the interaction potentials are not fully understood. Simulations are underway to better characterize more fully the factors influencing the growth mechanisms.

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