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Molecular dynamics investigation of the MBE growth of Si on Si{110}

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The crystal growth of Si{110} by deposition of single Si atoms from the gas phase is modeled by molecular dynamics simulations using an empirical potential. The bulk terminated Si{110} surface has easily accessible epitaxial sites for growth. However, we find the most stable adsorption site on the clean surface is a threefold coordinated site and not the epitaxial site. The adsorbed atoms in the threefold coordinated sites tend to destabilize atoms in the original surface layer. This causes interlayer diffusion in which the destabilized surface atoms move up into the growing layers. We find that even though the formed crystalline structure is perfect with no vacancies, the atoms from the original surface layer move to the top of four added layers and as much as one third of the original surface atoms migrate into the forming layers. Simulations also reveal that there is a chain mechanism whereby atoms in non-epitaxial sites are pushed into epitaxial positions when a row is nearly full.

1. Introduction

The ability to grow single defect-free layers of crystals makes it possible to develop semiconductor devices on an extremely small scale with very specific electronic properties. The high degree of control over the crystalline growth process that is necessary for atomic scale design often requires not only precision instrumentation but an intimate understanding of fundamental mechanisms of atomic motion on the surface. One important experimental method of controlling crystalline growth is molecular beam epitaxy (MBE) in which atoms are emitted from an oven into an ultrahigh vacuum chamber and deposited on a substrate which is held at constant temperature.

Considerable attention, both experimental and theoretical, has been given to understanding the MBE growth of silicon. The emphasis, however, has been on the {111} and {100} surfaces. The {111} surface has the fascinating (7×7) reconstruction, and the {100} surface is the predominant experimental growth surface. There is now growing interest in the {110} surface [1–6]. In particular, Si/Ge strained layer superlattices have been grown on the {110} surface of Si and Ge substrates [1,2], GaAs{110} has been layered on Si{110} [3], and Si{110} has been used as a template for $CoSi_2$ layers [4]. The {110} surface has been used in these cases because of some of its unique features. Si/Ge superlattices grown on Si{110} show nearly complete confinement of optical phonons to either the Si or Ge layers [5] and show quasi-direct band gaps that are not possible in the {100} or {111} orientations [6]. However, the quality of the interface between the Si and Ge layers affects the strain in the layers, thus changing the electronic energies and the confinement of phonons [5]. Intermixing is prominent when the superlattices are grown or annealed at or above 600 K [1]. In the case of GaAs on Si{110}, the growth is 2-dimensional which results in a greatly reduced number of dislocations from the number present in layers grown on Si{100} or Si{111} [3]. The latter show 3-dimensional growth patterns with island formation. Si{110} and {100}

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show ballistic transport across the interface with $CoSi_2$ while Si{111}, on which most $CoSi_2$ studies have concentrated, does not. These results indicate that Si{110} is important and significantly different from Si{111} and Si{100} such that further theoretical study is warranted. In this work we use molecular dynamics (MD) simulations to examine the atomic deposition and layer growth processes of Si on Si{110} with the aim of understanding the mechanisms of epitaxial growth and of the interlayer mixing of atoms during growth.

To initiate the MD simulations a model of the {110} surface is needed. Scanning tunneling microscopy studies of the Si{110} surface have shown that there is a long range (16×2) reconstruction [7–9]. However, the resolution is not sufficient to determine the individual atomic positions. There appear to be relatively large, almost bulk-terminated, terrace regions separated in height by the bulk layer separation distance. Since relatively little has been investigated on the microscopic nature of this surface, we have chosen the bulk-terminated Si{110} surface as shown in fig. 1 for our initial studies. The bulk terminated Si{110} surface can be described as a series of valleys and ridges where each valley or ridge consists of a zig-zag row of atoms. Each atom in the bulk is bound to its two neighbors in the same zig-zag row and one atom below and one atom above. For surface atoms, the atom above is missing, resulting in a radical orbital. The simulations in this study consist of deposition of Si atoms from the gas phase onto this bulk terminated surface using the molecular dynamics approach.

Molecular dynamics simulations of the early stages of MBE growth on the {111} and {100} surfaces have been successful at proposing sites for deposition and reaction mechanisms [10–15]. In addition, the temperature dependence of the growth processes have also been examined [10–13]. In this work we not only explore the dynamical features of the epitaxial growth such as surface temperature and coverage dependencies, but also analyze the detailed atomic motions that give rise to these dependencies. Of importance is that the most stable adsorption site is a threefold coordinated site, not the epitaxial position on the radical orbital. This proposed adsorption into the

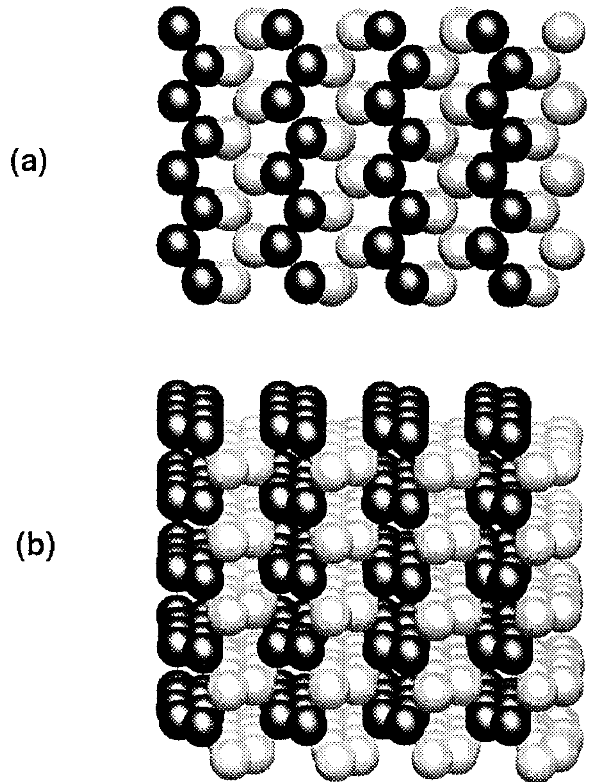

Fig. 1. Si{110} crystal used in the simulations. (a) Top view. (b) Side view. The top layer and all odd numbered layers are shaded dark and all even numbered layers are shaded light.

threefold site is in agreement with the theoretical calculations of adsorption energies on Si{110} [16,17]. We find that an occupied threefold coordinated site [16] strains the surface and thus alters the energetics of adatom adsorption near it. Thereby it enhances the motion of atoms out of the surface making possible interlayer diffusion during the growth. As much as one third of the original surface atoms are found to have migrated into the growing interface during the simulation.

We present the work in this paper as follows. In the second section we discuss the methods and parameters used to simulate the dynamic behavior of atoms during deposition on the {110} surface and the energetics of adsorption. In the third section we report and discuss the results of the simulation. Finally in the last section we conclude

and discuss the implications of the results of this study.

2. Description of the calculation

The goals of the simulations of the Si atom deposition on the Si{110} surface are to determine the overall characteristics of the growth, the growth mechanisms of both epitaxial and amorphous layers, and the final equilibrium configurations of the individual atoms. Because the atomic positions and momenta are determined as a function of time, the method of molecular dynamics simulations is a powerful approach for achieving these goals. The first part of this section describes the MD approach and the details of the simulation. The method for calculating static energetics of equilibrium geometries and barriers for activated dynamics is discussed next.

In the MD simulations the gas-phase atoms were randomly deposited on a slab of substrate atoms held at a given temperature. The dynamics of the substrate and the deposited atoms were evolved by solving the classical equations of motion using forces derived from realistic interaction potentials. The resulting differential equations were integrated in finite short time steps of approximately 10^{-15} s for 1–10 ns (1 ns = 10^{-9} s). Adatoms were added approximately every 20 ps (1 ps = 10^{-12} s) resulting in a deposition of 32 adatoms every 0.64 ns. In a simulation cell of the size of 32 atoms per layer thus the growth rate in the simulation was about 1 layer per 0.64 ns, which was sufficiently slow to accommodate the highly exothermic adsorption of atoms and the atomic motions that result from the adsorption. However, the simulation deposition rate is many orders of magnitude faster than the experimental deposition rate of about one layer per minute. Simulations on the scale of the experimental deposition rate would have required prohibitive amounts of computation time. Despite the discrepancy in film deposition rates, we believe that the MD simulations can give insight into the MBE growth process.

The realism of any MD simulation rests on the quality of the interaction potential from which the interatomic forces are derived. The many-body Tersoff [18] potential has been used successfully for growth studies on the Si{100}(2 × 1) surface [13] and for studies of Si–Ge heterostructures [19,20]. We thus chose to use the Tersoff Si potential for these simulations of the MBE growth on the Si{110} surface. We note that, however, the simulation temperatures reported in this work do not correspond to the real experimental temperatures [13]. The melting temperature for Si in MD simulations using the Tersoff potential [18] is found to be about 3200 K [13], whereas experimentally bulk Si melts at about 1683 K [21]. At the melting point, therefore, the simulation temperature is about twice the realistic experimental temperature. At lower temperatures the relationship between the simulation and the experimental temperatures may not be a linear one. Thus throughout this work we refer strictly only to the high and low temperature effects, where the relative changes are with respect to the simulation temperatures.

The initial crystal used for deposition was a slab of atoms with periodic boundary conditions imposed in the horizontal (x, y) directions. There were 10 layers of atoms with 32 atoms per layer for a total of 320 atoms as shown in fig. 1. The atoms in the bottommost layer were anchored in position with the next four layers forming a stochastic region. The atoms in this region experienced forces due to the Tersoff interaction potential as well as external frictional forces. The magnitude of the friction constant was proportional to the temperature of the system [22]. As the temperature of the system rose (fell) due to physical or chemical interactions between the substrate and the deposited atoms, the magnitude of the frictional forces on the atoms in the stochastic region were increased (decreased) proportionally to damp high (low) temperature oscillations of these atoms. The top five layers and all deposited atoms moved only due to the influence of the Si interaction potential. A complete simulation consisted of the deposition of 128 atoms (the number required to form four layers) from the gas phase onto the slab described above. Adatoms were directed at random locations on the surface from a distance above the surface

such that initially the adatoms were positioned just beyond the potential cutoff distance of all the other atoms. The initial kinetic energy of the incident atoms was near thermal and after each deposition the system was equilibrated for a period of 20 ps.

One useful way to interpret the results from the MD simulations is to construct a potential

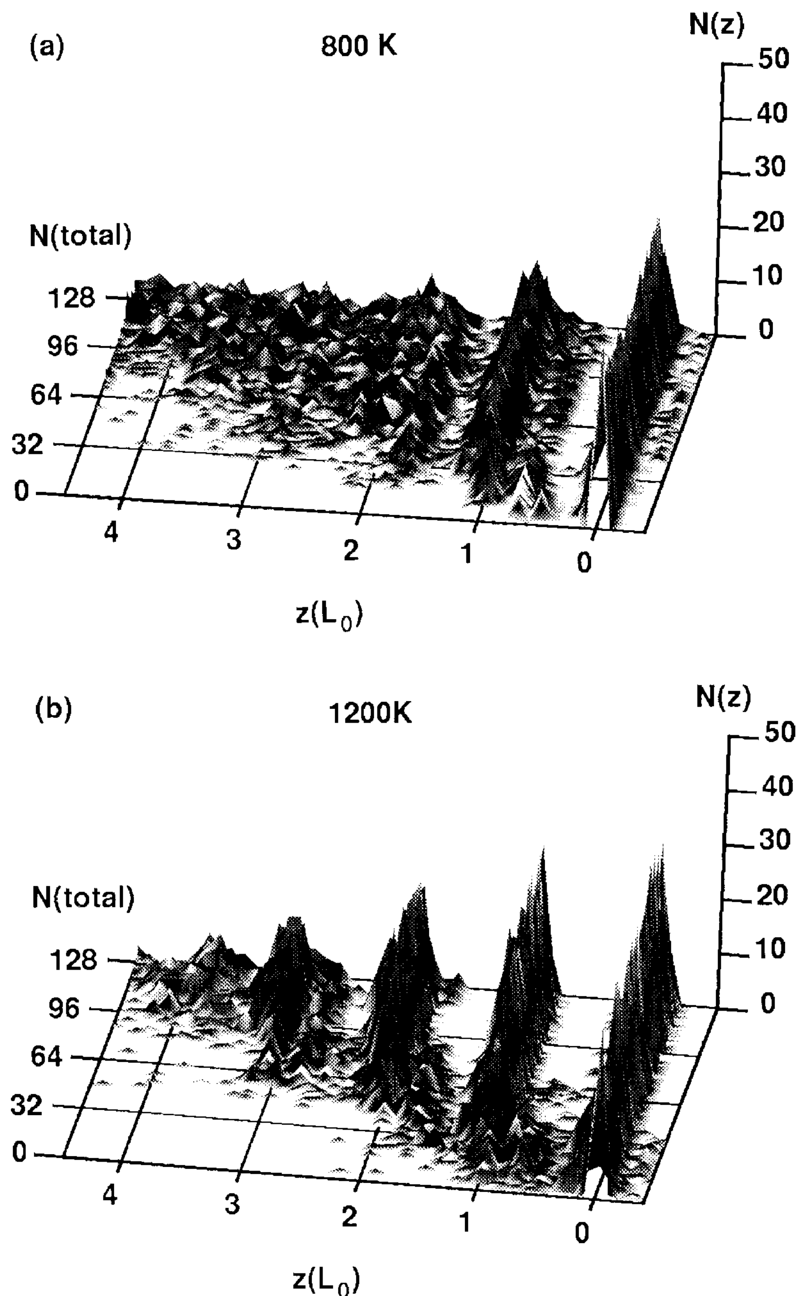

Fig. 2. Number density as a function of height, z and time, t. The number density and the time are in units of atoms added, and z is in units of L_0 (1.9 Å). The temperature is (a) 800, (b) 1200, (c) 2000, and (d) 2500 K, respectively.

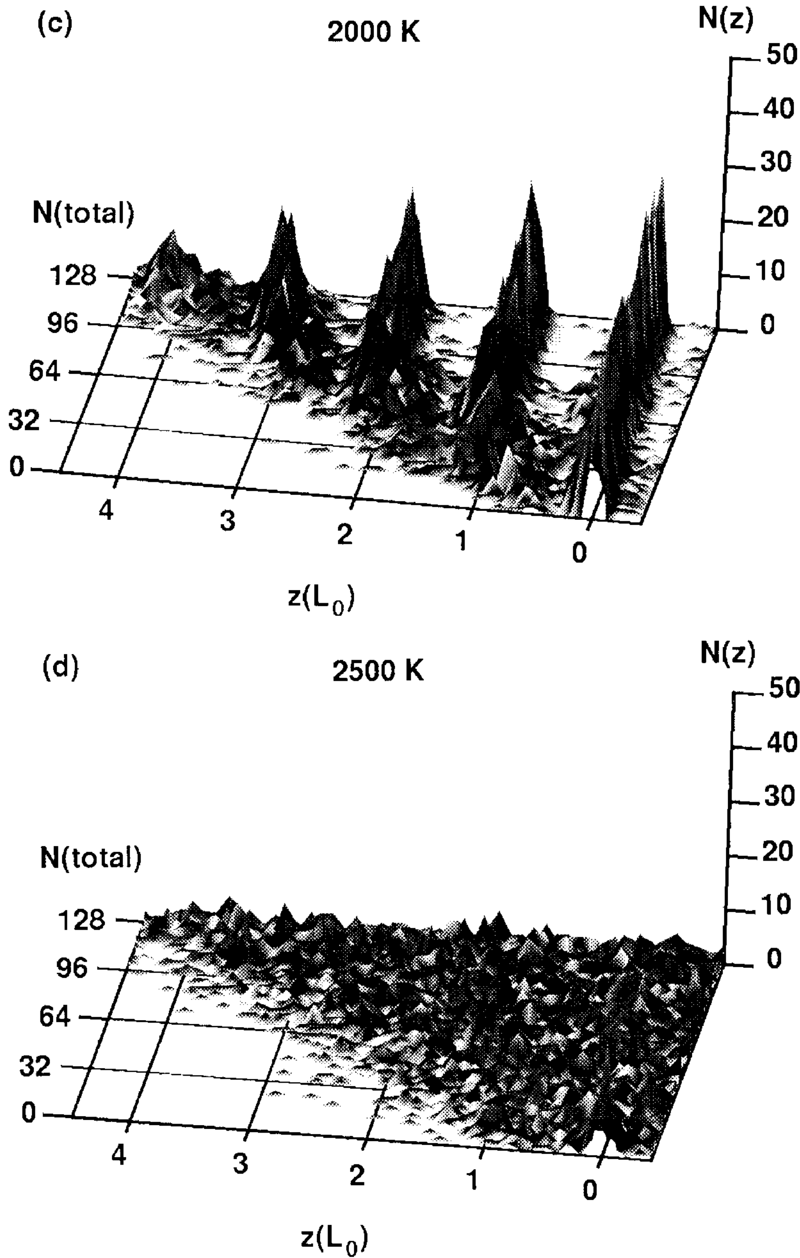

Fig. 2. Continued.

energy surface for a single adatom on the Si{110} surface and analyze the activated dynamics that may be occurring during the initial stages of the deposition [23–25]. This surface was constructed by dividing a unit cell on the Si{110} surface into 40×20 grid points in the x- and y-directions. An adatom was placed at the (x, y) position, its motion constrained along the z-direction (normal to the surface) above the crystal. The entire system was then equilibrated at 1200 K by MD simulations for about 1 ps to allow the adatom to move into the vicinity of the z-value where the

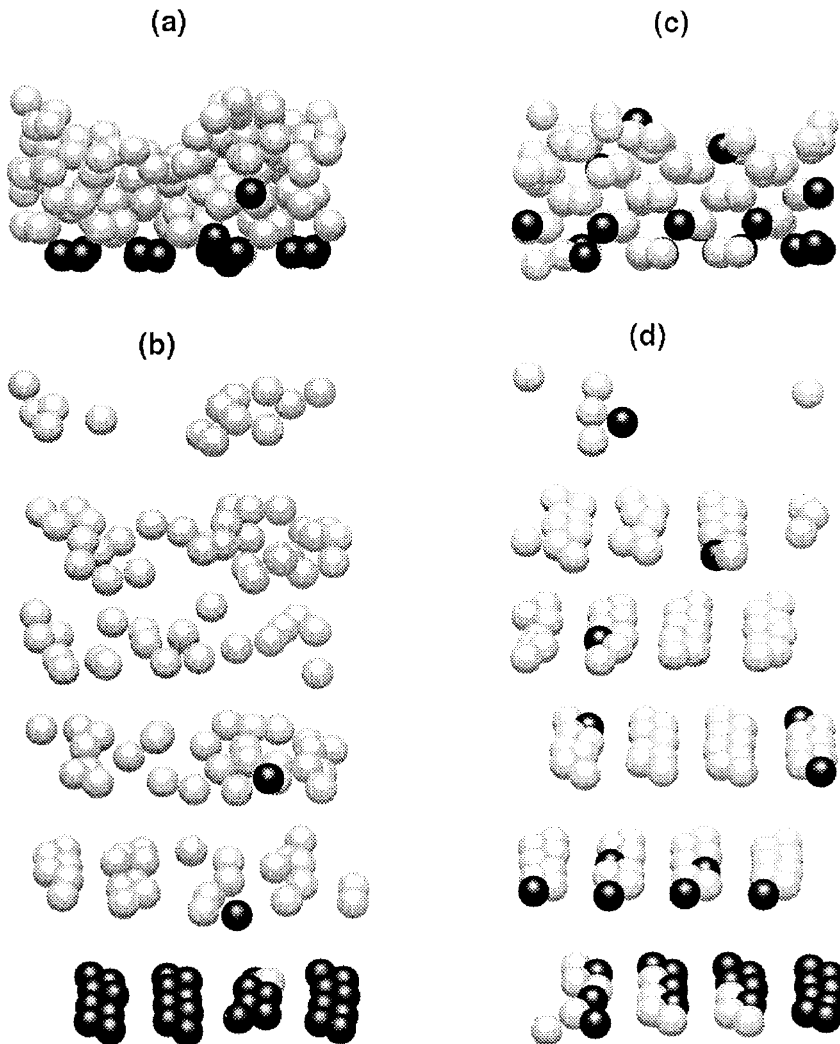

Fig. 3. Interlayer mixing of atoms during deposition. The original surface atoms are dark, and the adatoms are light. (a) 800 K, side view of original surface layer and the adlayers. (b) Same as (a) only the vertical axis has been expanded. (c) 2000 K, side view of original surface layer and the adlayers. (d) Same as (c) only the vertical axis has been expanded.

adatom–surface potential is a minimum. The kinetic energy was then slowly removed from the system by independently setting each velocity component of each atom to zero as the kinetic energy for that component passed through a maximum value. The finally quenched system thus is a minimum total energy configuration. We define the adsorption energy as the energy of the quenched crystal with the adatom adsorbed at the grid position minus the energy of the bulk-terminated crystal with the adatom at an infinite distance above the surface.

3. Results

The following section describes the results on the quality of epitaxial growth on the Si{110}

surface as a function of surface temperature. The atomic scale mechanisms leading to epitaxial film formation and interlayer diffusion are also discussed. We find that these latter phenomena can be explained in terms of the potential energy surface for single-adatom dynamics on the {110} surface.

3.1. Temperature effects on the quality of film formation

To assess the crystalline quality of the simulated systems, the number density of atoms, $N(z)$, is plotted versus the height, z, as shown in fig. 2. A perfect crystalline structure will exhibit a series of sharp peaks spaced at intervals of the bulk layer separation, L_0, where L_0 is 1.9 Å. In this graphical representation a third dimension, the evolution in time, has been introduced. For example, in fig. 2a the original surface layer is the peak extending from foreground to background at position 0. As time progresses (moving towards the background of the figure) Si atoms are added to the surface. Concurrent with the addition of atoms more layers form on the surface corresponding to moving towards the left in the figure.

Four temperatures were examined in this study and the number density profiles are shown in fig. 2. Concentrating first on the lower three temperatures, there is a distinct peak at position 0 that corresponds to the original surface layer. The first atoms that are added to the original surface adsorb at heights less than the interlayer spacing, suggesting that the initial adsorption sites might not be epitaxial. As more atoms are added to the surface, the first added layer becomes more well defined as evidenced by the sharp peak at position 1 and the lack of atom density between positions 0 and 1. This behavior is observed in subsequent layer depositions at 1200 and 2000 K, thus a nice crystalline film is produced. At 800 K, however, some of the initially deposited adatoms do not ever move into the epitaxial positions. Consequently, there are only few signs of a layered structure in the later deposited material and the film is more amorphous in nature. At 2500 K the original surface melts and consequently the entire deposited material remains noncrystalline. In summary, we have found that there is a finite simulation temperature range in which good crystalline growth occurs. As mentioned earlier we also note that the simulation temperatures are approximately a factor of two too high as compared to the realistic experimental temperatures [13].

The number density plots for 1200 and 2000 K show sharp peaks at correct layer positions indicating layer formation. However, one needs to observe the atomic positions to determine whether the layers are of the correct {110} structure, i.e. perfect crystalline character. Fig. 3 shows that indeed there is perfect {110} structure to the layers and also a significant amount of interlayer mixing due to diffusion. The explanation of the interlayer diffusion as well as the analysis of the initial adsorption close to the surface will be given in the next section.

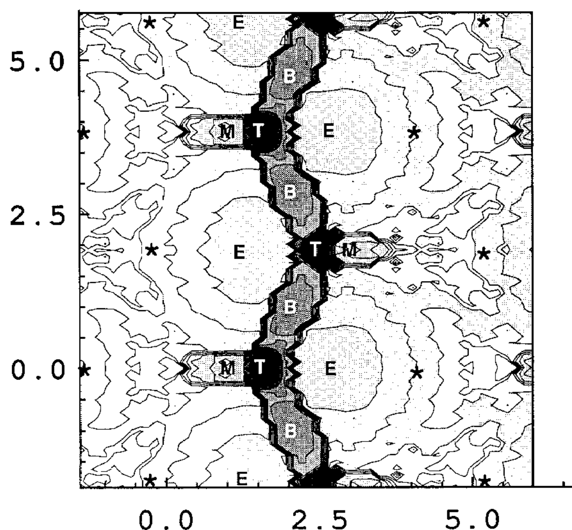

Fig. 4. Energy contour plot for one adatom on the clean Si{110} surface. The sites are denoted by letters. The asterisks denote the positions of surface atoms. The gray scale is such that darker intensity represents lower energies. That is, the T site is lower in energy than the E site. The axes are labeled in ångström units. The contour plot was determined by calculating energy values in two of the approximately eight symmetrically equivalent regions shown in the figure. Any asymmetry in the figure is due to not symmetrizing over the two sets of calculations.

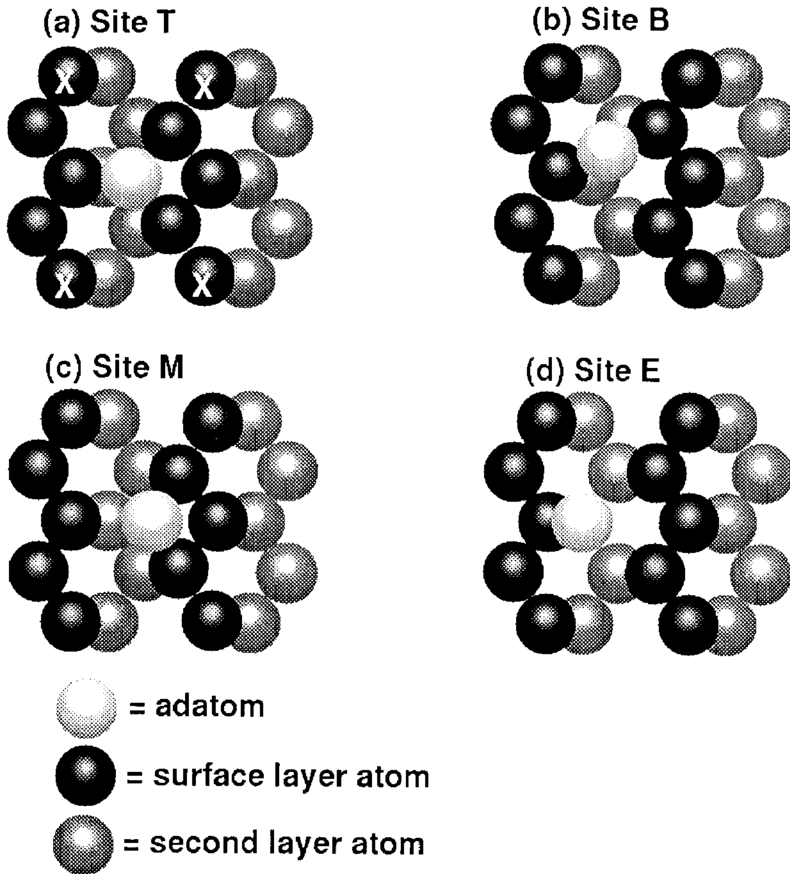

Fig. 5. Adsorption sites. (a) Threefold coordinated T site. The surface atoms that are most likely to migrate out of the surface as discussed in the text are denoted by X's. (b) Twofold coordinated B site. (c) Twofold coordinated M site. (d) Onefold coordinated epitaxial E site.

3.2. Potential energy of the surface

In order to understand the adsorption process and the interlayer mixing, we start by examining the simplest case of the energetics of adsorption of a single adatom onto a clean, bulk-terminated Si{110} surface. Shown in fig. 4 for two adjacent rectangular unit cells of the surface is the two-dimensional potential surface constructed as described above. There are four distinct adsorption sites (T, B, M, E) also shown in fig. 5 and whose characteristics are given in table 1.

Table 1
Energetics and positions of the local minima for a Si atom on a clean Si{110} surface

Site	Energy (eV)	Coordination	Height [a]		Activation energy [b] (eV)	Site [c]
			(Å)	L_0		
T	−4.35	3	1.0	0.53	0.6	B
B	−3.90	2	1.2	0.63	0.2	T
M	−2.77	2	1.4	0.74	< 0.1	T
E	−2.38	1	1.9	1.00	0.2	T, B

[a] Height relative to the original layer of surface atoms.
[b] Lowest activation energy to any of the adjacent sites.
[c] Site that corresponds to the lowest activation energy.

The energetics and height of the adatom above the surface correlate quite well with the coordination of each site. The epitaxial site, E, is only coordinated to one surface atom and is thus the least stable and is highest above the surface. The T site, on the other hand, is coordinated with three surface atoms and is thus the most stable and closest to the surface. The two twofold coordinated sites, B and M, are mid-way in both quantities. Of note is that even though the E site is the least stable of the four sites, it occupies the largest extent (70%) of the surface area. The prediction that the threefold coordinated T site is the most stable agrees with recent electronic structure calculations [16].

3.3. Adsorption dynamics

The adsorption dynamics on the Si{110} surface are strongly influenced by the low barriers to diffusion among the various sites (table 1). It appears in the simulation that the majority of deposited atoms land in the E site which is the site that occupies the largest surface area. However, the residence time is less than 1 ps, a short time even within the MD simulations. Thus in reality the dominant adsorption site on the clean surface is the T site. Since the T site position is about 0.5 L_0 above the original surface, peaks appear in the number density plots (figs. 2a–2c) between layers. This easy migration out of the radical orbital site (E) is in contrast to what is observed in MD simulations using the same potential on the Si{100}(2 × 1) surface [24]. In this latter case, diffusion from the radical site is not readily observed in the time scale of MD simulations.

Although the deposited atoms adsorbed into T sites, ultimately there was an epitaxial layer formation (figs. 2a–2c). Consequently the adatoms had to move back into the E sites. From an examination of figs. 4 and 5, it is apparent that adjacent T sites cannot be occupied. As the coverage of adatoms in one trough or valley approached 1/3 to 1/2 of a monolayer, the deposited atoms started adsorbing into B sites or migrating down the valley to an accessible T site. (We did not observe diffusion between valleys in the time scale of our simulations.) Ultimately at about 1/2 of a monolayer, an incoming atom has only E sites accessible. Occupation of the E site, at this point, shifts the other atoms towards occu-

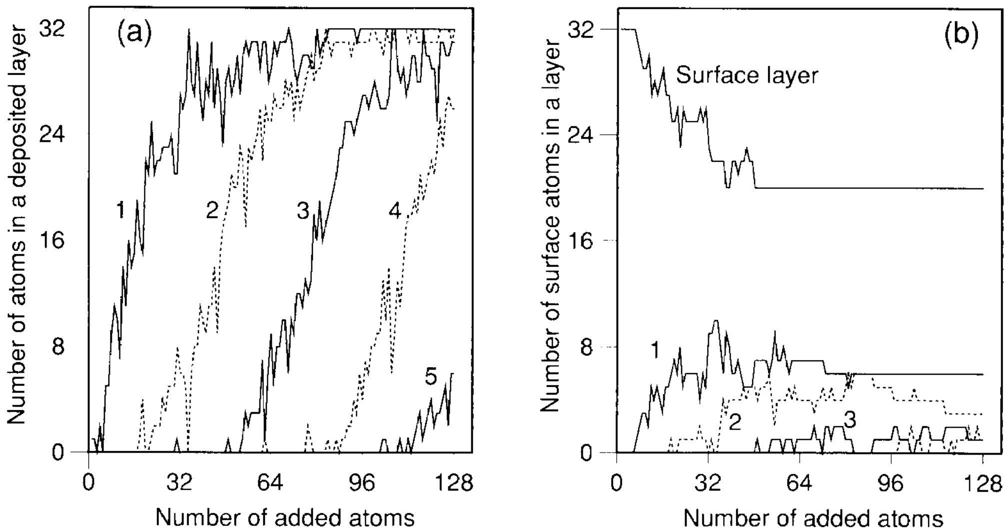

Fig. 6. Layer growth characteristics versus number of atoms added to the system for the 2000 K simulation. (a) Number of atoms in each layer. Here we have defined a layer from the perfect position down 0.58 to up 0.42 L_0 in order to make sure that adsorbing atoms in T sites are counted with the layer above. (b) Subsequent fate of the 32 atoms in the original surface layer.

pying B and E sites rather than T and B sites. Finally one atom adsorbs into an E site causing a cascade down the valley putting all adatoms into E sites. Due to the limited size of our crystallite, we observed this cascade for only up to 5–6 atoms. This process is thermally activated, and consequently it was not observed in the MD simulations at the lowest temperature.

3.4. Layer formation and interlayer diffusion

Even within the short time scale of our calculations layers grow nearly one full layer at a time, that is, a new layer does not begin to form until the underlying layer is about half complete. This is largely due to the multitude of adsorption sites in each valley and the ease of diffusion along the valley. Fig. 6a shows the progress of growth in each layer as a function of how many adatoms are added for the 2000 K simulation. In the figure it is apparent that the layers fill to a full 32 atoms, and that a new layer does not begin to fill until the current surface layer contains about 20–24 atoms. In the simulation we observed that the atoms in a newly forming layer are adsorbed on completed rows and not on the incomplete part of the surface. Note that our simulations are restricted in the deposition rate and the starting substrate size. Consequently we are limited in our ability to simulate any diffusion of surface atoms from newly forming rows to areas of incomplete rows in the previous layer.

The phenomenon of interlayer diffusion appears in our simulations and grows in importance as the simulation temperature increases from 800 to 2000 K. The interlayer diffusion is clearly shown in fig. 3d where the original surface atoms (shown in black) are distributed throughout the first four added layers. This phenomenon is characteristic of the simulations on the Si{110} surface and deserves further explanation.

We examine the details of the diffusion process by analyzing the atomic motions associated with an exchange of atoms between layers. Three major characteristics are apparent. First, the event responsible for the diffusion of an adatom between two layers occurs as a two step process. Initially, an atom in an already formed layer moves into the growing layer immediately above it. Subsequently the vacancy in the underlying layer is filled by a downward migrating adatom. The second characteristic is that the exchange of atoms between layers occurs only at the surface layer and not below. We did not observe atoms diffusing down any further than the surface layer that the adatoms encountered upon adsorption. However, by the stepwise manner of the diffusion, atoms are found several layers above their starting point. The third major characteristic is that the event of upward atomic motion correlates positively with the occupation of T sites and not directly with adsorption of an adatom. The motion of an atom in the underlying surface layer occurs in locations where there are several adatoms in T sites and approximately 1/4 to 3/4 local occupation density. There is no exchange in a locally clean surface. The most common surface atom to migrate has no adatoms bound to it from above, and has two surface neighbors each bound to an adatom in a T site. Adatoms in T sites [16,17] destabilize the surface atoms by causing strain in the surrounding surface. Fig. 5 shows the position of the surface atoms most often observed to migrate upward relative to an occupied T site. After the upward migration of the surface atom, another adatom can move into the original surface. This interlayer diffusion mechanism also allows for local lateral migration of atoms. The average characteristics of this diffusion are shown in fig. 6b, which is described below.

The migration of the 32 atoms of the original surface layer during the 2000 K simulation is traced as a function of the number of atoms added in fig. 6b. After the addition of ~ 40 atoms there is no change in the number of original surface atoms remaining in the original layer and after the addition of ~ 70 atoms there is no change in the first layer profile. The explanation for this is in fig. 6a where the total number of atoms in each added layer is shown as a function of the number of adatoms. Initially there is only growth in the first layer. After about 16 adatoms or 1/2 of a layer, the second layer begins to fill. At approximately 35 adatoms the first layer is nearly full and at ~ 75 adatoms the second layer is full. The points correlate well to those where

the original surface atoms stop migrating out of the corresponding underlayer. Thus we conclude that once a layer is completely covered, there is no migration out of it.

We note that the interlayer diffusion of the surface Si atoms into growing Si overlayers is not experimentally significant because in the final structure there is no distinction between the surface and the deposited Si atoms. In heteroepitaxial growth of Ge on Si{110} surface a temperature and coverage dependent alloy formation at the interface of the epitaxially grown heterostructure is noticed [1]. The observed interlayer diffusion of Si atoms into the growing structure provides a mechanism for such an alloy formation at the interface of the growing heterostructure. We note that such a mechanism, if indeed confirmed through similar simulation of Ge heteroepitaxy on the Si{110} surface, is due to the kinetic effects during the growth and not due to any lattice mismatch strain driven effects in the final equilibrium structure [6].

4. Conclusions

The MD simulations using an empirical potential of MBE growth on Si{110} show that it is characterized by layer-at-a-time growth and that the formation of each layer follows a three step mechanism. The initial 1/3 of the layer formation on a clean surface is dominated by adsorption of adatoms into stable threefold coordinated sites (T sites). During the second phase (1/3 to 2/3 layer formation), many adatoms adsorb into bridge sites and many T sites adatoms migrate to B sites. During this phase a considerable amount of interlayer exchange of atoms occurs due to the strain on the surface from the T site adatoms. During the final 1/3 layer formation, the MD simulations have identified a chain mechanism whereby adatoms adsorb into epitaxial positions and force other adatoms into crystalline positions as well. Little interlayer diffusion occurs during the final 1/3 of a layer is being filled and no interlayer diffusion occurs after a layer is covered by a crystalline layer. We have identified an interlayer diffusion mechanism where the adsorption into T sites destablizes atoms in the surface below. The surface atoms can easily move into the growing layer and thus new adatoms can fill the vacancy in the underlying layer. Even though an empirical potential has been used, these MD simulations suggest novel migration mechanisms for investigation by ab initio methods.

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