

Atomistic simulation of silicon beam deposition

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The mechanisms controlling low-energy (10–100 eV) beam deposition of silicon onto a relaxed (111) silicon substrate have been studied using a molecular-dynamics technique. The atomic interaction was modeled using a many-body empirical potential so that the effects of the covalent Si—Si bonding could be accurately included. 10-eV silicon atoms with near-perpendicular incidence were studied to determine the energy-loss mechanism resulting in capture and subsequent diffusion of excess vibrational energy away from the impact point. Shallower angles of incidence (5° – 30°) were studied for beam energies of 20–100 eV. For incidence angles less than an energy- and orientation-dependent critical value, a new phenomenon of "surface channeling" is observed, in which the trajectory of the incoming particle is steered parallel to, and roughly 2 Å above, the surface of the substrate by inelastic interaction with the surface atoms. The rate of energy loss in surface channeling trajectories is very slow, so that ranges of thousands of angstroms along the surface are possible. The phenomena observed in low-energy beam deposition offer considerable promise for precision control of the growth of nonequilibrium semiconductor structures.

I. INTRODUCTION

Devices with a more critical dependence on physical structure than had previously been required are currently of great interest. Examples of such structures include superlattices, strained-layer systems, devices with ultrathin layers, such as single quantum wells, and so on. The performance of such devices can be very sensitive to the presence of defect structures. Since defects often correlate with substrate temperature, one approach to reducing defect density is to optimize the growth temperature. However, this optimization involves balancing competing processes: If the temperature is too low, defects associated with unannealed configurations will remain, whereas if the temperature is too high, thermally induced defects will appear. For some systems an adequate window of temperatures exists between these two limits, but this is not always the case.

A nonequilibrium approach to reducing defects in the growth process is to keep the bulk of the structure relatively cool during deposition while supplying the additional excitation needed to grow high-quality material through some specific interaction with the surface. One proposed technique is low-energy ion-beam deposition, in which experimental studies have recently begun.¹ As the beam energy must be larger than the energy of adsorption of a silicon atom onto a silicon surface (a few eV) to significantly change the adsorption dynamics from those of conventional deposition processes, the perpendicular and near-perpendicular atomic-beam deposition of 10-eV silicon atoms onto, and the grazing-incidence interaction of 20–100 eV silicon atoms with, a silicon (111) surface has been simulated. The methodology is first described, and then the results of the simulations are discussed.

II. SIMULATION METHOD AND INTERACTION POTENTIAL

Molecular-dynamics techniques have been used with considerable success to simulate the microscopic response of atomistic systems to a given set of conditions.² In molecular dynamics the classical equations of motion for an assembly of interacting particles are integrated numerically, resulting in a complete classical description of the system over the integration period. In the current simulations, we are generally concerned with length scales of less than 10 nm, several hundred atoms, and time scales less than a picosecond. These restrictions make the problem easily accessible to conventional molecular-dynamics techniques.

Proper description of the Si—Si bonding interactions is an important factor in these low-energy simulations. In the simulation of high-energy (many keV) ion-substrate interactions, the ion-atom potential is taken as spherically symmetric and purely repulsive, since the kinetic energy is so much larger than the binding energy.³ These approximations cannot properly be applied in the very-low-energy regime with which we are currently concerned, especially when concerned with materials which form highly directional covalent bonds. Several many-body empirical potentials which describe, with various regimes of applicability, the bonding of silicon have recently been introduced.^{4–7} The potential recently introduced by Dodson,⁷ following earlier work by Tersoff,⁶ which provides a useful and accurate global description of the structural energetics of silicon, is used here.

In the Dodson potential, the structural energy is the sum over the asymmetric potential Φ_{ij}

$$E = 0.5 \sum_{i,j} \Phi_{ij}, \quad (1)$$

where the pairwise potential Φ_{ij} has a form similar to a Morse potential, but contains a many-body interference term B_{ij}

$$\Phi_{ij} = f_{ij} (Ae^{-\lambda_1 r_{ij}} - B_{ij}e^{-\lambda_2 r_{ij}}), \quad (2)$$

where A , λ_1 , and λ_2 are fitting parameters and f_{ij} is a radial cutoff term active near 3 Å. The influence of neighboring atoms on the bonding interaction is embedded in the many-body interference term B_{ij} , where

$$B_{ij} = B_0 \exp[-(z_{ij})^\eta / b] \quad (3)$$

and

$$z_{ij} = \sum_{\substack{k \\ k \neq i, j}} [f_{ik} / f_{ij}]^4 \exp[4\lambda_2(r_{ij} - r_{ik})] \\ \times [c + \exp(-d \cos \theta_{jik})]^{-1}. \quad (4)$$

The parameters of the potential were fit, using a simulated annealing technique, to the lattice constant and cohesive energy of various high-density phases of silicon, the bulk modulus of bulk silicon, and the bond length and binding energy of the Si_2 dimer. The parameter values obtained using this procedure, in units of Å and eV, are

$$\begin{aligned} A &= 1614.6, & b &= 3.4785, \\ B_0 &= 155.08, & c &= 0.8543, \\ \lambda_1 &= 2.7793, & d &= 3.9588, \\ \lambda_2 &= 1.3969, & \eta &= 0.6207. \end{aligned}$$

The resulting potential accurately describes the structural energetics of silicon over a broad range of configurations.⁷

The kinetic energies used in the present simulation are large enough that suspicion may be raised concerning the behavior of the potential at small r , since it is based on a data set primarily concerned with deformation of the outer electron shell. As the momentum transfer in an individual scattering even rises, the inner shell structure will produce harder-core behavior than predicted by the Dodson potential. The error resulting from this factor must be evaluated in two different regimes, near-perpendicular beam deposition and the predicted surface channeling of more grazing incidence angles. In the first case, there will be large momentum transfer in individual scattering events. In this regime, the resulting errors are rendered acceptable by limiting the beam energy to 10 eV. When considering grazing angles of incidence, the accuracy of the potential at small r is unimportant, since the trajectories of interest result from glancing interactions with the surface in which the vertical momentum is absorbed by gentle inelastic interactions with many surface atoms. We therefore have reasonable confidence in the present use of the Dodson potential, but emphasize that (at least) an additional hard-core repulsive term would be needed to extend the description to problems requiring treatment of larger momentum transfers.

Proper description of the physics of low-energy beam deposition of silicon requires the use of such a many-body potential. The most time-consuming step in the

molecular-dynamics integration scheme is thus to determine the forces acting on each particle by differentiation of the many-body potential. In order to limit the difficulty of computation, we have chosen the Schofield method,⁸ a simple, although stable, low-order integration routine requiring only one force calculation per time step. The finite difference equations for this scheme are

$$x(t+dt) = x(t) + v(t)dt \\ + [4f(t) - f(t-dt)](dt)^2/6, \quad (5a)$$

$$v(t+dt) = v(t) + [2f(t+dt) + 5f(t) \\ - f(t-dt)]dt/6, \quad (5b)$$

where $v(t)$ and $f(t)$ are the x components of the velocity and force at time t (the mass is set equal to one here). The resulting algorithm, using a time step of 0.5 fsec, has proven satisfactory for the class of problems considered here.

III. ATOMIC BEAM DEPOSITION OF SILICON

In considering the adsorption phenomena which may affect the atomic beam deposition of silicon, two dynamical properties are of particular interest. The first is the simple description of adsorption dynamics of the incident atom, including such factors as sticking coefficient, depth of penetration, location of adsorbed atom (surface, interstitial site, etc.), and sputtering of substrate atoms. These quantities allow one to describe the direct consequences of atomic beam growth. In addition, however, the excess kinetic energy and momentum of the atomic beam must be carried away by substrate lattice excitation if the incoming particle is to stick. This excess energy provides a local and short-lived region of vibrational excitation which may serve to selectively anneal nearby metastable configurations which arise during the process of growth. It is therefore important to determine characteristic time, length, and energy scales driving this nonequilibrium annealing process.

A. Near-perpendicular beam incidence: Adsorption

The incoming atoms from normal or near-normal 10-eV silicon beams stop very quickly (0.05–0.1 psec). Since lattice vibrations will travel no more than a few Å in this period, the adsorption sites of the incident atoms were determined through studies on a small substrate, namely a 4×4 cell on the (111) surface six atomic layers thick (96 atoms total). Since the duration of the simulation is small enough that phonons will not propagate over the dimensions of the substrate, free boundary conditions can be used at all surfaces without disturbing the adsorption dynamics. The surface of the Si(111) substrate is relaxed, but unreconstructed. The surface relaxes in by about 0.7 Å, reducing the energy of the system by 0.12 eV/surface atom, in good agreement with *ab initio* calculations.⁷ The silicon atom from the incoming beam is assigned a random initial position above the (111) surface, and the evolution of the system is then calculated using the molecular-dynamics procedure described above. Sets of 30 trajectories were analyzed to determine trends in the

deposition of atoms directed perpendicular to the surface, with a 60° angle of incidence and surface projection parallel to the $[110]$ surface vector (a bulk channeling direction), and with a 60° angle of incidence and surface projection parallel to the $[1\bar{2}0]$ surface vector (not a bulk channeling direction). In normal incidence, 70% of the incident atoms either come to rest in an interstitial position between the first and second double atomic layers or substitute for an atom in the first double layer by knocking the substrate atom into an interstitial location; the other 30% come to rest on the surface. For the 60° $[1\bar{2}0]$ case, 50% of the incident atoms become interstitials between the first two double atomic layers. The other 50% come to rest on the surface, usually after skipping perhaps 10 \AA from the initial impact point along the surface. For a 60° angle of incidence parallel to a bulk channeling direction, the results are similar (60% penetrate, 40% surface). In this case, however, the incident atoms do not travel across the surface before they stop. It appears that the bulk channeling directions have little influence on the penetration of incident silicon atoms in this energy range. All incident atoms stick to the substrate, and no substrate atoms sputter off, indicating a sticking coefficient of one, within the limitations inherent in examining a finite number of trajectories.

B. Near-perpendicular beam incidence: Surface excitation

Propagation of excess vibrational energy away from the impact point is now considered. Since the excitation front will travel with sonic velocities, the time scale which can be treated in the calculation is limited by the interaction of the excitation front with the substrate boundaries. A larger substrate is used for these relaxation studies so that adequate time scales can be reached. The silicon substrate used consists of a 6×8 cell eight atomic layers in thickness on an unreconstructed but relaxed (111) free surface, with a total of 384 atoms. This structure is large enough that reflected phonons cannot disturb the dynamics of the incoming beam atom in the 0.2 psec duration of the calculation, and thus, free boundary conditions are again used safely. All other features of the calculation are identical with those described earlier.

The kinetic energy and momentum of an incident atom is almost entirely transferred to the substrate lattice within 0.02 psec of the initial interaction. The energy and momentum first couple to substrate atoms near the impact point by collision-induced momentum transfer, and then transport away from the impact point via phonons. This process results in a transient spike of high vibrational excitation near the impact point, which may serve to activate modifications of the atomic configuration near the impact point. In order to evaluate this possibility, characteristic time, length, and energy scales of the transient spike were determined by calculating the radial (relative to the impact point) kinetic energy density and radial dependence of the average kinetic energy per substrate atom (local "temperature") as a function of time after impact.

A typical set of results are presented in Figs. 1 and 2, which show the time evolution of, respectively, the radial kinetic energy density and the local "temperature" for the

first 0.2 psec of the simulation. The 10-eV atom has normal incidence. It begins to interact with the substrate atoms at $t=0$ [Figs. 1(a) and 2(a)]. At 0.02 psec, 80% of the initial kinetic energy of the incident atom has been transferred to the substrate, divided almost evenly between kinetic and potential lattice energy. At this time the excitation has only affected atoms surrounding the impact site; the radius of the excitation front is roughly 4 \AA [Fig. 1(b)] and the average kinetic energy per atom in this

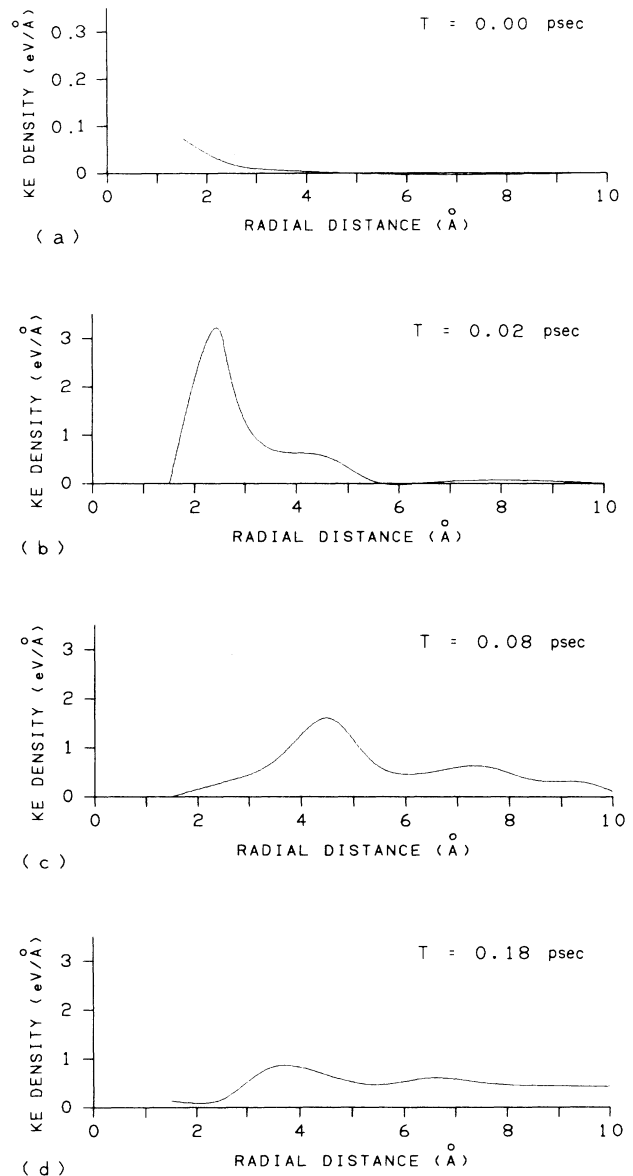


FIG. 1. Time evolution of the radial kinetic energy (KE) density as a function of distance from the impact point of perpendicularly directed 10-eV silicon atom incident on a silicon (111) surface. The kinetic energy in a spherical shell is calculated and normalized to units of $\text{eV}/\text{\AA}$. (a) is at $t=0$, (b) is at 0.02 psec, (c) is at 0.08 psec, and (d) is at $t=0.18$ psec. The excess energy resulting from the initial collision radiates from the impact site at near-sonic velocity.

region is about 0.3 eV [Fig. 2(b)]. The next set of graphs [Figs. 1(c) and 2(c)] describe the system at 0.08 psec. Here the excitation front has advanced to nearly 9 Å radius. This corresponds to a front velocity of 83 ± 20 Å/psec, which is remarkably (and, to some extent, coincidentally) similar to the sound velocity of 83 Å/psec. The large peak near 4.5 Å is a signature of a relatively long-lived local mode which slowly radiates energy into the

substrate. Detailed analysis of the time evolution of this mode reveals that the initial amplitude corresponds to an excitation of several eV, and that the local mode radiates its energy to the rest of the lattice with a time constant of about 0.08 psec. Finally [Fig. 1(d)] at 0.18 psec, the radial kinetic energy density, save for the diminishing influence of the small radius local mode, is nearly constant at 0.5 eV/Å past 15 Å radius. Consistent with this, the average kinetic energy per atom [Fig. 2(d)] continues to decrease roughly as r^{-2} beyond the local neighborhood of the impact point.

C. Grazing incidence: Trajectories of 20–100 eV Si atoms

The case of grazing beam incidence (3° – 30°) with energies of 20–100 eV is considered next. For grazing angles, the principal interaction with the substrate takes place by interaction with many substrate atoms, rather than through one major collision. This allows consideration of higher-beam energies without leaving the regime of applicability of the Dodson potential. The generic results in this regime of incidence angle and beam energy are rapid adsorption, trajectories which bounce off of the substrate, or long-range surface transport (denoted surface channeling). We consider grazing beam incidence onto a long thin silicon substrate which has an unreconstructed but relaxed (111) surface, about 12-Å wide and 80-Å long (in the [100] direction), is 4 atomic layers in thickness, and totals 320 atoms. This is large enough that reflected phonons do not disturb the dynamics of atoms from the incoming beam, as the atoms move rapidly enough to leave the disturbance behind. The silicon atom incident from the atomic beam is assigned an initial position, direction, and velocity. In all cases, the initial trajectory is oriented with the projection of the velocity onto the surface collinear with the surface [100] vector, so that the particle travels primarily along the long direction of the substrate. The evolution of the resulting system of 321 atoms is then calculated as before. The simulation is continued until the incoming particle bounces from the surface, is adsorbed onto the substrate, or falls off the edge of the substrate through surface channeling (typically a few tenths of a picosecond).

Results of a typical simulation run appear in Fig. 3. The incoming silicon atom had a kinetic energy of 40 eV and an initial angle of incidence of 10° relative to the surface of the substrate. In the figure, the response of the substrate to the impact of the atom is ignored, and the substrate atomic positions shown are simply the initial positions. (The substrate response is of course included in the molecular-dynamics simulation.) As the particle approaches the substrate, it begins to interact with the surface atoms. The kinetic energy increases slightly as the atom is attracted to the surface, but the interaction quickly turns repulsive and the particle bounces from the surface. However, the interaction with the surface atoms is sufficiently inelastic (because of phonons removing momentum from the impact site rather than the electronic effects which dominate in collisions with larger momentum transfer) that the rebounding particle does not escape from the lattice, but rather is trapped between the attrac-

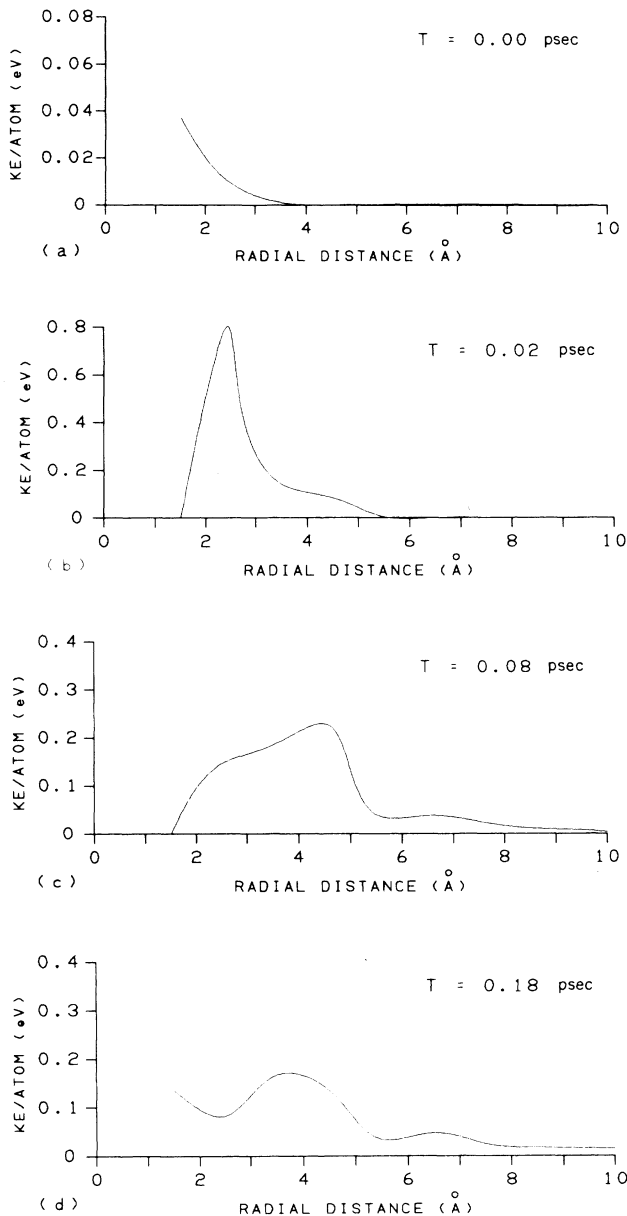


FIG. 2. Time evolution of the average kinetic energy per atom resulting from the impact of a perpendicularly directed 10-eV silicon atom on a silicon (111) surface as a function of distance from the impact point. (a) is at $t=0$, (b) is at 0.02 psec, (c) is at 0.08 psec, and (d) is at $t=0.18$ psec. The large residual kinetic energies at small (2–4 Å) radius are due to a local breathing mode with a time constant of 0.08 psec.

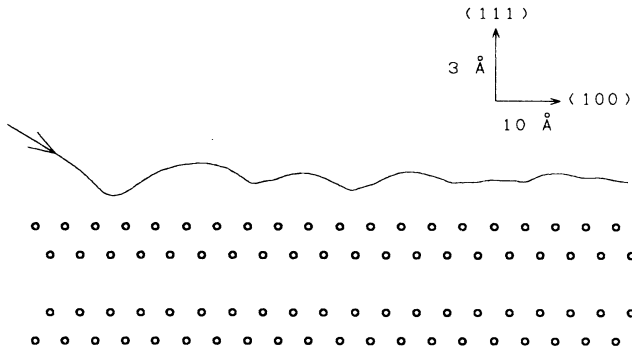


FIG. 3. The surface channeling trajectory of an energetic silicon atom above an unreconstructed silicon (111) surface. The incoming atom initially has a kinetic energy of 40 eV and an angle of incidence of 10° . The perpendicular momentum of the incoming atom is lost to the substrate through inelastic interactions, and the resulting trajectory is essentially parallel to, and about 2 Å above, the surface of the substrate. Evaluation of the rate of energy loss indicates that the surface channeling range for this 40-eV atom is several thousand Å.

tive and repulsive interactions with the surface of the substrate. The vertical oscillations in these competing fields damp out quickly as the atom undergoes further inelastic interaction with the substrate through phonon generation, and eventually settles down to motion nearly parallel to and about 2 Å above the surface of the substrate. In this mode, further loss of kinetic energy is extremely slow, and ranges of thousands of angstroms (on perfect surfaces) are possible.

D. Surface channeling trajectories

The behavior seen in Fig. 3 and described above is a general feature of low-angle beam-surface interactions in this energy range. We call this phenomenon "surface channeling," in analogy to the more conventional bulk channeling. In bulk channeling, a high-energy ion is steered along the symmetry directions of a lattice by the combined effect of the repulsive potentials of the atoms making up the lattice. The analogy in surface channeling is that the competition between the long-range attractive potential and short-range repulsive potential generated by the surface of the substrate serves to produce a potential well which guides the incoming atom along the surface, once the vertical momentum is lost to the substrate. The [100] direction seems particularly favorable on the (111) silicon surface, but surface channeling should also occur along other surface symmetry directions at more glancing angles.

The phenomenon called surface channeling described above must not be confused with the low-angle-trajectory focusing surface scattering described by Thompson and co-workers,^{9,10} or with the near-surface channeling mechanism proposed by Sizmann and Varelas.¹¹ In the first case, sometimes called surface semichanneling, orientations exist which focus the incoming beam onto a second-layer row of atoms, whereupon strong reflection from the surface with characteristic angular dependence takes

place. In the second case, the beam atoms actually penetrate the surface and channel within the bulk material near the surface, sometimes emerging again when dechanneling takes place. In both cases, the principal interaction with the substrate takes place below the surface layer, and transport does not take place above the surface. By contrast, in the surface channeling mechanism proposed here, the principal interaction is inelastic momentum transfer through generation of impact-generated bulk phonons, and transport occurs *above* the substrate surface, which is never penetrated. A similar type of trajectory is predicted to result from electronic effects by Ohtsuki *et al.*¹² They find that the motion of an incident ion produces a dynamical polarization of the valence electrons in the substrate, resulting in a small (≈ 10 eV) surface potential which can trap a grazing ion near the surface in a kind of skipping motion. Although the source of the beam trapping is completely different than that described here, it is interesting that similar effects result both from electronic and vibrational interactions with the substrate.

It is interesting to consider the effect of different initial conditions on the trajectories of incoming atoms. The initial location of the particle does not have a strong influence on the surface channeling phenomenon. We cannot rule out the possibility that there may be impact points on the surface which are particularly unfavorable for surface channeling, but such points were not found in the current work, in which roughly 100 trajectories were studied. It is clearly safe to say that, at a given beam orientation and kinetic energy, the appearance (or not) of surface channeling is a generic behavior, occasional special cases notwithstanding.

For a given initial beam energy, there is a critical angle θ_c below which we see surface channeling and above which either the particle bounces off or rapidly absorbs onto the surface (see sample trajectories in Fig. 4). Surface channeling quickly vanishes when the critical angle is exceeded. Note that, as the critical angle is exceeded, the lowest-energy atoms (20 eV) always undergo abrupt adsorption [Fig. 4(a)], whereas higher-energy (40 and 100 eV) atoms always bounce off [Fig. 4(b)]. The higher-energy atoms are expected to stick or penetrate for sufficiently steep angles, which suggests that there is a second critical angle ψ_c separating scattering off the surface from deposition onto the substrate (see Fig. 5).

The dependence of the critical angle on the initial energy of the beam is described next. We have performed a large number of simulations at 20, 40, and 100 eV in order to identify the critical angles (respectively 18° , 10° , and 5°) for each initial energy. These figures tell us that the perpendicular momentum, which must be carried away via inelastic interaction with the substrate, is a weak function of beam energy. More precisely, the critical perpendicular velocity is

$$V_p = 20.5 + 336/E_b \quad (6)$$

where V_p is in Å/psec and E_b is the beam energy in eV. This relation implies that the initial inelastic interaction with the surface removes similar amounts of perpendicular momentum regardless of the total kinetic energy of the incoming atom, allowing extrapolation of the critical con-

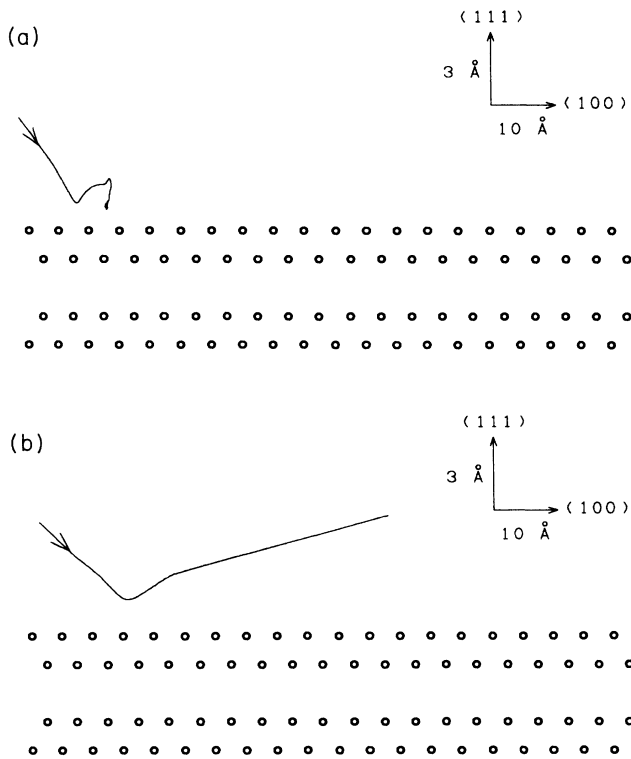


FIG. 4. Atomic trajectories not resulting in surface channeling. (a) Initial kinetic energy of 20 eV, angle of incidence of 20°. Adsorption occurs immediately following the first collision with the surface. (b) Initial kinetic energy of 40 eV, angle of incidence of 12°. The incoming particle scatters immediately from the surface.

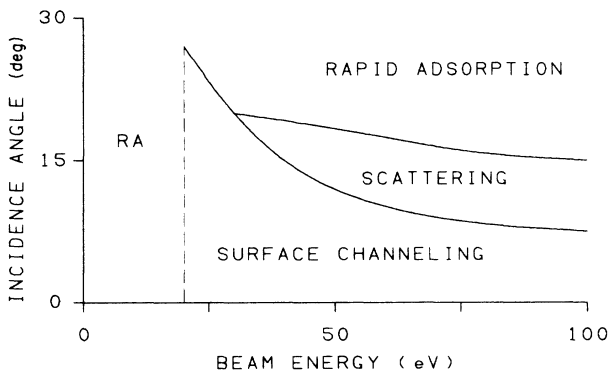


FIG. 5. Incidence angle vs beam energy phase plane for Si atoms incident on the Si(111) surface. Incoming atoms with either low kinetic energy or large angle of incidence will quickly become localized and adsorb at the surface (this region is marked RA for rapid adsorption). If the energy is above roughly 20 eV and the angle of incidence is sufficiently small, the atom will be steered into a surface channeling trajectory. At somewhat higher energies and intermediate incidence angles, the incoming atom scatters off the surface and does not stick.

ditions to higher energies. The above information is summarized in an incidence angle versus beam energy phase diagram (Fig. 5).

Finally, the rate of energy loss experienced by a particle in a surface channeling trajectory is of interest. This can be evaluated directly from the computed trajectories by numerical differentiation. Upon doing so, the rate of energy loss is found to be nearly linear in kinetic energy of the surface channeling atom; in this energy range,

$$\partial E / \partial X = 0.000154E - 0.0193, \quad (7)$$

where E is in eV and X is in Å. Clearly, this relation cannot be extrapolated far outside of this energy range, but it does allow estimation of the total surface channeling range along the surface as a function of initial beam energy. Crude estimates reveal that the surface channeling ranges will be thousands of Å for the higher-energy atoms. Direct calculation for the 20-eV atoms show that the linearity of the energy-loss relation fails badly for smaller energies, and a surface channeling range of around 40 Å is found before adsorption for these atoms, compared to perhaps 1000 Å as predicted by Eq. (6). It is possible that the effect of thermal motion on the substrate atoms could strongly affect the trajectory and rate of energy loss of a surface channeling particle. It is straightforward to include thermal substrate motions into the calculation, and such calculations are currently in progress. Preliminary results indicate that, at 400 K, the stability of the trajectories is not upset, and that the energy-loss rate is not drastically altered, although it is increased perhaps by a factor of 2.

IV. DISCUSSION

Let us first summarize the case of perpendicular or near-perpendicular incidence of 10 eV Si atoms on the unreconstructed Si(111) surface. In normal incidence, 30% of the incident atoms come to rest on top of the surface, whereas 70% penetrate into the top double layer and stop in interstitial sites. At an incidence angle of 60°, 50–60% of the incident atoms penetrate and stop in interstitial sites, while the remainder form a new layer on the surface. Thermal diffusion should eventually bring the interstitials to the surface, but this requires long times compared to our current simulation. When the beam orientation is parallel to a [120] surface vector, the incident atoms which remain on the surface first skip perhaps 10 Å along the surface from the initial impact point. When the orientation is along a [110] surface vector (the bulk channeling direction), those atoms remaining on the surface do not skip before adsorption. A small region near the impact point experiences very strong excitation and forms a short-lived ($\tau \approx 0.08$ psec) local mode which radiates the energy of the incident atom to the rest of the lattice as phonons. The lattice excitation (and accompanying distortion) beyond about 10 Å from the impact site will be insufficient to anneal metastable states. In no case were incident atoms seen to bounce off the substrate, nor were substrate atoms sputtered off.

In the case of grazing incidence, the most interesting result is prediction of surface channeling trajectories. In

surface channeling the competition between the long-range attractive potential and short-range repulsive potential generated by the surface of the substrate serves to produce a potential well which guides the incoming atom along the surface. For a given initial-beam energy, there is a critical angle θ_c below which we see surface channeling and above which either the particle bounces off or rapidly absorbs onto the surface. The [100] direction seems particularly favorable for surface channeling on the relaxed Si(111) surface, but it should occur along other surface vectors at more glancing angles. In a surface channeling trajectory on this idealized surface, loss of kinetic energy is extremely slow, and ranges of thousands of angstroms (on perfect surfaces) are possible.

The atomic beam adsorption processes described here offer several mechanisms which may lead to high-quality epitaxial growth. One is the formation and subsequent thermal annealing of near-surface interstitials. This produces a dense and locally distorted near-surface region which is likely to heal into a perfect epitaxial layer through thermal migration of the interstitial atoms. Since these interstitial atoms need not diffuse long distances to reach the surface, the healing suggested above should be a quick process, allowing high rates of deposition. Another mechanism is strong vibrational excitation of the region

near the impact of the incident atom, which will provide a nonthermal mechanism through which metastable defect structures may be eliminated. Finally, the surface channeling trajectories offer the possibility or preferentially transferring energy into badly placed surface atoms, resulting in benign growth on good crystal combined with selective removal of physisorbed impurities and improperly placed adatoms. Extending our current studies into actual simulations of crystal growth has not been possible because of the long-time scales involved. However, it seems clear that low-energy atomic beam deposition offers several nonthermal mechanisms for influencing the quality of epitaxial crystal growth. Either simple low-energy beam deposition or a combination of beam deposition with more conventional molecular-beam epitaxy seem to be reasonable possibilities for high-quality epitaxial film growth in semiconductors.

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