Calculated Schwoebel barriers on Si(111) steps using an empirical potential

S. Kodiyalam, K.E. Khor and S. Das Sarma

Department of Physics, University of Maryland, College Park, Maryland 20742-4111

(Submitted to Physical Review on July 14th 1995, Resubmitted on November 27 1995)

Motivated by the recent investigations on instabilities caused by Schwoebel barriers during growth and their effects on growth or sublimation by step flows, we have investigated, using the Stillinger-Weber potential, how this step edge barrier arises for the two high symmetry steps on 1×1 reconstructed Si(111). Relative to a barrier of 0.97 ± 0.07 eV on the surface, we find additional (Schwoebel) barriers of 0.61 ± 0.07 eV and 0.16 ± 0.07 eV for adatom migration over the [211] and the [112] steps respectively. The adatom potential energy is found to be strongly correlated with that derived from the local geometry of atoms on the adatom-free surface or step edges. This correlation preserves a strict correspondence between the barrier determining features in the spatial variation of the adatom potential energy and the same derived from the local geometry for the Si(111) surface and the [211] step. It is therefore argued that the Schwoebel barrier on the [211] step is robust i.e. a feature that would survive in more satisfactory ab initio or tight binding calculations. Using a diffusion equation for the adatom concentration the relevance of the barrier to electromigration of steps has been explored. Data from such experiments on Si(111) has been used to place an upper bound on the Schwoebel barrier and a lower bound on the electromigration force.

PACS numbers: 68.35Fx, 68.35Ja, 68.35Bs, 68.35Md
I. INTRODUCTION

The Schwoebel barrier was originally introduced in the context of step motion \cite{1} as the additional barrier for adatom diffusion over a step edge from the upper to lower terraces. It was argued that such a barrier results in an anisotropy in adatom diffusion into the step edge - the diffusion from the lower terrace being greater. This anisotropy was found to drive an arbitrary distribution of step spacings towards a uniform distribution during growth of a vicinal surface. \cite{1} Later, it was pointed out by Villain \cite{2} that this growth by step flow is stable only on a sufficiently vicinal surface with possible instabilities setting in during the growth of a flat (singular) surface. The dynamical morphology of a singular surface growing under the influence of a schwoebel barrier is a subject of great current activity. \cite{2,3} While the eventual fate of growth on a flat surface in the presence of such extra step edge barriers is still being discussed \cite{3,6,7}, it is now well accepted that Schwoebel barriers lead to coarsening in the evolving surface morphology under nonequilibrium growth conditions, producing mounds, pyramids and facet-like angular structures on the growing surface. Recent experimental studies of nonequilibrium growth on the Si(111) surface have produced somewhat contradictory \cite{8,9} results, and the specific role of Schwoebel barriers for nonequilibrium Si(111) growth is unclear at the present time.

The current study is primarily motivated by observations of another instability: As was pointed out by Schwoebel and Shipsey \cite{1}, an anisotropy favoring diffusion into the step edge from the upper terrace (possibly due to larger barriers for diffusion from the lower terrace) results in a step pairing instability during the growth of a vicinal surface. In recent experiments similar direct-current induced reversible step-bunching instabilities have been observed during sublimation of the high temperature 1×1 phase of Si(111). \cite{11,12}. Here, we report on a calculation of the Schwoebel barrier for the two high symmetry vicinal steps on 1×1 Si(111) using the empirical Stillinger-Weber potential. \cite{13} The importance of the Schwoebel barrier in the context of the electromigration experiments has also been explored by modeling the barrier as affecting the boundary conditions to the diffusion equation for
II. EMPIRICAL POTENTIAL CALCULATIONS

The use of the Stillinger-Weber potential in this study has been motivated by its successful application in previous studies of bulk and liquid silicon [13], the Si(100) surface and steps on this surface [15]. Barriers on the Si(100) surface and on single and double height steps on this surface have also been calculated using this potential. [18–20] Although this potential fails to reproduce the correct energetics of the Si(111) surface configurations with adatoms, [16] it has been used here since features that follow purely from the changes in the adatom coordination number are expected to be robust i.e. these features survive even if the details of the empirical potential used change. Such features are expected to survive in more satisfactory ab initio or tight binding calculations. The calculation here is followed by an attempt to identify such robust features.

To determine the diffusion barriers the adatom potential energy has been mapped as a function of the \((x, y)\) position of the adatom (in the (111) plane) for the Si(111) surface (Fig. 2(a)), the \([\overline{2}11]\) step (Fig. 2(d)) and the \([\Pi2]\) step (Fig. 2(g)). The three-fold and reflection symmetry of the Si(111) as shown in Fig. 1 implies that steps running along directions with equal \(\theta\) are identical. It has been shown in a previous study [21] using the Stillinger-Weber potential that an alternative configuration of step-edge atoms with some of the upper terrace atoms rebonding to atoms in the lower terrace gives a lower step energy for the \([\overline{1}12]\) and \([101]\) steps. However, such a configuration has not been considered here since it has also been shown that it gives rise to step-step interactions an order of magnitude larger than experimental estimates. [21] Neglecting such rebonded configurations, all the intermediate low symmetry steps \((0^0 < \theta < 60^0)\) have been shown to have a higher step energy. [21] In other words, diffusion barriers have been calculated for those steps whose interactions are not larger than experimental estimates and whose step energy is a local minimum as a function their orientation \(\theta\). The adatom potential energy \(V\) has been computed as the difference in

adatom concentration used to interpret these experiments [14].
the minimum potential energy of the system with the adatom at infinity (non-interacting) and the same with the interacting adatom.

Standard molecular dynamics (MD) procedures of integrating Newton’s law (with dissipation to reduce temperature) and the steepest descent equations have been used to determine the minimum potential energy of the system. \[21\] These routines determined the adatom potential energy to an accuracy of $10^{-4}$ eV. The $(x,y)$ coordinates of the adatom are fixed during the integration process. The system consisted of a certain number of bilayers of Si(111) in an MD cell with the surface lattice constants $a_1$ and $a_2$ along its $x$ and $y$ directions respectively (see Fig. 1). Three of the bottom bi-layers are fixed at bulk lattice coordinates throughout the calculation. In simulations on the Si(111) surface with six additional (movable) bi-layers it was found that changing the adatom’s $(x,y)$ position from a deep minimum lead to the shearing of the entire surface in the $xy$ plane towards the adatom. As this made the $(x,y)$ position of the adatom relative to the surface ill defined further simulations on the surface as well as the step configurations were carried out with atoms at the $(x,y)$ boundaries also fixed at positions corresponding to the adatom-free but relaxed configurations. The regions in the (111) plane explored in all cases were “centrally” located i.e. maximally away from the boundaries so that finite size effects are minimized. System size dependence in $V(x,y)$ was initially explored for the Si(111) surface to determine the optimal system size. It was found that changing the system size from four lattice constants in the $x$ and $y$ directions (including the boundary of fixed atoms) with three movable bi-layers to six lattice constants in the $x$ and $y$ directions with six movable bi-layers changed (reduced) the adatom potential energy (at the minima, maxima and saddle points) by $< 10^{-2}$ eV. As an error bar of $\pm 10^{-2}$ eV was estimated to be smaller that the accuracy needed for this study all the simulations were carried out with the smaller system size - the size in the $y$ direction being extended to $4\frac{2}{3}$ and $4\frac{1}{3}$ lattice constants for the $[\overline{2}11]$ and $[\overline{1}12]$ step configurations respectively so that periodic boundary conditions could be applied to create vicinal steps. Since the bulk terminated Si(111) surface and $[\overline{2}11]$ step configurations do not relax under the Stillinger-Weber potential, with the system sizes chosen here their corresponding surface
and step energies are reproduced exactly. However, the $[\overline{1}12]$ step configuration is different from the bulk terminated structure due to the $2\times1$ reconstruction at the step edge. With the system size chosen here it’s step energy is reproduced to within $4\times10^{-4}$ eV/$a_1$. \[21\]

The MD procedures began with initial configurations for each $(x,y)$ position of the adatom corresponding to the relaxed adatom-free structures. The $z$ coordinate of the adatom was chosen to be equal to that obtained in the final configuration during simulation with the adatom in the immediate neighborhood of the point $(x,y)$. For the step configurations $V(x,y)$ was determined from behind to the front of the step edge. These procedures for determining $V(x,y)$ were found necessary for the $[211]$ step configuration since other methods such as an arbitrary initial $z$ coordinate for the adatom or determining $V(x,y)$ from the front to behind the step edge lead to the adatom relaxing into configurations in which it displaces an atom near the step edge and/or moves into the bulk. Symmetries in the $(111)$ plane were exploited to reduce the size of the regions in which the adatom potential energy needs to be computed. Therefore for the Si(111) surface only a sixth of the surface unit cell was explored. For this case $V(x,y)$ was computed on a triangular grid - the sides of the triangle coinciding with the high symmetry directions with the distance between neighboring grid points being $\frac{a_1}{3}$. An interpolation scheme respecting the symmetries on the surface was used to determine the features of $V(x,y)$. For the $[211]$ and $[\overline{1}12]$ step configurations reflection symmetry about the $y$ axis ($\perp$ to the step edge) reduced the width of the region (along the step edge) explored to a length of $\frac{a_1}{2}$ and $a_1$ respectively. For these configurations $V(x,y)$ was determined on a rectangular grid with the distance between neighboring grid points being $\frac{a_1}{16}$ and $\frac{a_1}{30}$ along the $x$ and $y$ axis respectively. With the step edge in the middle, the length of the region explored was $1\frac{2}{3}a_2$ and $1\frac{1}{3}a_2$ for the $[211]$ and $[\overline{1}12]$ steps respectively. This was to enable a new interpolation scheme (respecting the symmetries of the step configurations) applying periodic boundary conditions along the $x$ axis to do the same along the $y$ axis of the region explored. On comparing the potential energy of the adatom on the Si(111) surface to that far away from the $[211]$ step edge errors due to the finite grid sizes, the interpolation schemes and possibly effects due to being close to the boundary of fixed atoms
were recognized. These errors are conservatively estimated to be ±0.05 eV. Since this is much larger than the errors due to finite size effects it is assumed to be the error bar in the potential energy. Barrier values being differences in these potential energies are therefore estimated to have an error bar of ±0.07 eV.

III. RESULTS AND DISCUSSION

The results are shown in Fig. 2. The global minimum of the adatom potential energy $V$ occurs on the $H_3$ site ($m_1$) on the Si(111) surface (Fig. 2(b)) where the adatom potential energy is -3.31 eV. This is a significant fraction of the bulk energy per atom: -4.34 eV. The relevant saddle point for $H_3 \leftrightarrow H_3$ transitions is $s_1$ (close to the $T_4$ cite which is a local minimum) where the potential energy is -2.34 eV. Thus the barrier to diffusion on the surface is 0.97±0.07 eV. These results are consistent with previous studies (using the same potential) on surface energies of configurations with adatoms [16] as well as a study of diffusion on the Si(111) surface. [22] The barriers to diffusion between the minima along the step edges are slightly smaller than the barrier on the surface - apparently inconsistent with previous work [34] showing that step edge fluctuations are (predominantly) due to attachment/detachment of adatoms from the terrace and not due to diffusion of atoms along the step edge. In this study the Schwoebel barrier has been defined to be difference between the maximum adatom potential energy (along the path on which this is a minimum) as it moves into the step edge from the global minimum on the upper terrace far away from the step edge and the same for the $H_3 \leftrightarrow H_3$ transitions on the Si(111) surface. In other words it is the difference in the adatom potential energies at the barrier determining saddle point on the step configurations and the same on the free surface ($s_1$). With this definition the Schwoebel barrier cannot be negative. From Fig. 2(e) (Fig. 2(h)), for the $[211]$ ($[\bar{1}12]$) step the barrier is determined by $s_3$ ($s_5$) where the adatom potential energy is -1.73 eV (-2.18 eV) - implying a Schwoebel barrier of 0.61±0.07 eV (0.16±0.07 eV). Growth on Si(111) is therefore expected to produce
moundlike structures with facets consisting (predominantly) of $[\overline{2}11]$ steps. However, the experiments of Yang et al (temperature = 275±5°C) instead show facets with $[\overline{1}12]$ steps. This discrepancy may be due to the presence of the 7×7 reconstruction.

It must be noted that the Stillinger-Weber potential has been tuned only to the properties of the bulk diamond and liquid structures of Silicon and not to any surface or step properties. As mentioned previously it does not produce the correct energetics for the Si(111) surface configurations with adatoms [16] as compared to ab initio calculations. [23–25] Therefore an attempt has been made to identify the robust features of this study: Features following from changes in the coordination number of the adatom. This idea is supported by the observation that the reconstruction energy of the Si(100) surface calculated using the Stillinger-Weber potential [26] (0.85 eV) agrees with ab initio calculations [27] (0.84 eV). The Tersoff and Dodson empirical potentials also give this energy to be of the same order of magnitude. [26] The Stillinger-Weber also reproduces the correct order of energies of the $[\overline{2}11]$ and $[\overline{1}12]$ steps (per step edge atom these values are 0.72 eV and 0.62 eV respectively [21]) as well as the presence of rebonding at the $[\overline{1}12]$ step edge as compared to tight binding calculations (per step edge atom these values are 0.70 eV and 0.38 eV respectively [17]).

During reconstruction, the coordination number of atoms (on the (100) surface and $[\overline{1}12]$ step edge) changes from two to three. It is therefore expected that features following from such a change in coordination number are not artifacts of the empirical potential used. Here, the adatom energy recomputed without additional relaxation of other atoms due to the presence of the adatom is assumed to be a good measure of the coordination number. Although this measure is very similar to the actual adatom energy $V(x,y)$, it helps to identify features that follow from the geometry of atoms (locally around to adatom) on the relaxed adatom-free surface or step edges. Features that do not change significantly due to additional relaxations in the presence of the adatom are expected to be robust. The adatom potential energy $V_{ad}(x,y)$ has therefore been recomputed with other atoms fixed at positions corresponding to the relaxed adatom-free structures. These results are shown in Fig. 2(c) for the Si(111) surface, Fig. 2(f) for the $[\overline{2}11]$ step and in Fig. 2(i) for the $[\overline{1}12]$
Similarities in the contour plots of $V$ and $V_{lg}$ suggest a strong correlation between them. This correlation is evident from the linear relationship between $V_{lg}$ and $V$ (Fig. 3). The lines in Fig. 3 are best fits to $V_{lg}(x, y)$ vs $V(x, y)$ which were explicitly computed at the grid points. There is no repetition of points that are equivalent due to the symmetries of the relevant configurations. Further, for the step configurations, the length of the region along the $y$ axis corresponding to these plots is $\frac{1}{2}a_2$ on either side of the step edge. The rough configuration independence of the relationship between $V_{lg}$ and $V$ suggests that it is a characteristic of the [111] surface. A similar behavior may be true for the Si(100) surface and single height steps on it. In this case, borrowing the values of $V$ corresponding to the features (minima and saddle points) from previous work by Roland and Gilmer [18–20], and computing $V_{lg}$ for the same features here, it is found that $V_{lg} = (1.3 \pm 0.2)V + (1.2 \pm 0.5)$ for the Si(100) surface and $V_{lg} = (1.1 \pm 0.1)V + (0.6 \pm 0.3)$ for the combined data from the three single height steps.

### A. Relevance to electromigration experiments

Recent experiments on the electromigration of steps on Si(111) [11,12] can be reinterpreted in the presence of a Schwoebel barrier by modifying the boundary conditions to the diffusion equation for adatom concentration used previously by Stoyanov et al [14] to describe step bunching (see appendix A). The particular modification is to suppress the strength of the step as a source of adatoms onto the upper terrace relative to the same onto the lower terrace by a factor $e^\epsilon$ where $\epsilon = \frac{2E_s}{k_B T}$ with $E_s$ being the Schwoebel barrier. With this modification the equations for adatom concentration on a particular terrace has four length scales - the diffusion length $\lambda$ and the scale introduced by the electromigration force $f (=\frac{F}{k_B T})$ both of which are parameters entering the diffusion equation and two other scales $t_0$ and $t_1$ entering the boundary condition to this equation at the upper and lower terrace step edges respectively ($t_{0,1} = \frac{\beta n_e}{a^2 D n_e}$, $a^{-2}$ is the density of atoms in a terrace, $D$ is the diffusion constant, $n_e$ is the equilibrium adatom density and $\beta$ is the step kinetic coefficient - here the
Schwoebel barrier is modeled as making this parameter assume different values at the upper and lower terrace step edges. These are in addition to the scale introduced by the terrace width $W$. Since the modification is further designed to keep the total strength of the step as a source of adatoms a constant independent of $E_s$, $t_0 + t_1 = t$ - a constant independent of $\epsilon$ for fixed $k_0T$ (variation of $t$ with $E_s$ is included in the estimated range of $t$ ) with $\frac{t_0}{t_1} = e^\epsilon$.

The (linear) diffusion equation is then solved, with $n_e$ appearing in the boundary conditions as a “source”, to obtain the spatial variation of the adatom concentration.

Using the above solution the equations for the velocities of an array of steps with positions $X_i$ are developed - the step index $i$ increases in the step down direction which is also the positive $x$ axis. The time scale that enters these equations is the lifetime of an adatom $\tau_{lf}$.

These equations have the following form (see appendix A):

$$\dot{X}_n = \frac{\theta_e}{\tau_{lf}} \lambda [g_-(\epsilon, t\lambda, f\lambda, W_n, \lambda^{-1}) + g_+(\epsilon, t\lambda, f\lambda, W_{n-1}, \lambda^{-1})]$$

where $\theta_e = n_e a^2$ and the terrace width $W_n = X_{n+1} - X_n$. From the above, equations for the rate of change of the terrace widths can be obtained. Linear stability analysis of these equations around an average terrace width $w$ would predict when the step bunching instability occurs. The linearized equations may be written as follows:

$$\dot{\delta}_n = k_- \dot{\delta}_{n+1} + (k_- - k_+) \dot{\delta}_n + k_+ \dot{\delta}_{n-1}$$

where $\delta_n = W_n - w$ and $k_\pm = \frac{\theta_e}{\tau_{lf}} \lambda \left[ \frac{\partial g\pm}{\partial W} \right]_{W=w}$. The instability occurs if $k_+ - k_- > 0$ or equivalently (since $k_+ + k_- < 0$ for $w > 0$), when the anisotropy ratio $\rho = \frac{k_+}{k_-} < 1$. This analysis is similar to the work of Ghez et al [29] which includes an external flux with the electromigration force being absent.

The recent experiment of Williams et al on reversible step bunching on Si(111), which measures an “effective” anisotropy ratio $\rho_{eff}$ (near bunched steps) in the temperature range 1155-1215$^o$ C (this range includes the corrections due to the emissivity of the optical pyrometer used in the experiment [12]), can now be used to to determine an upper bound on $E_s$ ($E_s^u$) and a lower bound on $F$ ($F_l$) by solving the equation $\tau^{-1} = k_+ - \rho k_- = 0$. The solution
to this equation is obtained by estimating the parameters $w$, $t$ and $\lambda$ (in the temperature range of interest: 1155-1215° C) and then determining $f$ as a function of $\epsilon$. The estimates of the upper and lower bounds on $t$ and $\lambda$ are made conservatively - the range is made wide enough so as to include the “true value”. Experimental observations of Latyshev et al [11] show that around a temperature of 1200° C the step velocity varies linearly with the terrace width up to a width of 2 $\mu m$. A lower bound on the diffusion length $[32]$ of 0.5 $\mu m$ is obtained by reproducing this result using equation 1. This estimate is robust against large changes in the parameters $t$ and $f$. To make this estimate, $\epsilon$ is conservatively chosen to be zero. Further, to first order in $w\lambda^{-1}$, $g_+ + g_- = -w\lambda^{-1}$ - independent of $t$, $\epsilon$ and $f$. Therefore the magnitude of the slopes of the above curves correspond to the evaporation rates $r = \theta_e \tau_{lf}$. An estimate of the upper bound on $\lambda$ is obtained by estimating the diffusion constant $[32]$ $D$ (using $D = b^2 \nu e^{-E_a/k_b T}$, $b=3.84 \text{Å}$, $\nu=10^{13}\text{s}^{-1}$, $E_a=0.97\text{ eV}$ (calculated here)) and an estimate of the upper bound on $\tau_{lf} = \frac{n_e a^2}{r}$ (The temperature dependence of $r$ in the data from Latyshev et al [11] is consistent with the theory of Burton et al [30] (BCF) with an activation energy equal to the cohesive energy of silicon ($E_b=4.34\text{ eV}$)). The upper bound on $\theta_e$ is assumed to be 0.167 - the primary motivation for this is that it is measured to be $\approx 0.1$ around 900° C and its activation energy $E_n$, which is equal to $E_b - E_r$ ($E_r$ is the activation energy for $\tau_{lf}^{-1}$) from the BCF theory, is estimated to be negative since total energy calculations $[33]$ predict smaller surface energies for silicon surfaces with adatoms as compared to the 1×1 surface thereby making $E_r > E_b$. The specific value of 0.167 is chosen as it corresponds to the density in any $\sqrt{3} \times \sqrt{3}$ configuration of adatoms wherein all the floating bonds on the 1×1 substrate are saturated by bonding with the adatoms - at higher densities adatom interactions are expected to be significant. This bound is therefore required here as a measure of internal consistency in the analysis since the diffusion equations used correspond to free adatoms. The upper bound on $\tau_{lf}$ is calculated using this value of $\theta_e$. As the variation in $n_e$ has been argued to be small $[32]$ $E_n \approx 0$ and $E_r \approx E_b > E_a$. The estimate of the upper bound on $\lambda$ ($=(D\tau_{lf})^{1/2}$) is therefore made at the lowest temperature of interest and is equal to $\approx 70 \mu m$. The upper bound used in this study is $\approx 7$ times this
value, making \(0.5 \mu m \leq \lambda \leq 0.5 \times 10^3 \mu m\).

The estimate of the range of \(t\) is obtained from the range of \(\lambda\), the measured \(r(T_2)\) and \(\theta_e(T_1)\) and the relation between \(\beta_s = \beta_0 + \beta_1\) and the measured step mobility \(\Gamma(T_1)\) \(T_1\) corresponds to 900° C and \(T_2\) corresponds to temperatures of interest). At the same temperature, \(\beta_s = \frac{\Gamma(T_1)}{a}\) (see appendix B). From a model of attachment-detachment at the step edges (see appendix B) the temperature and \(\theta_e\) dependences of \(\beta_s\) is determined: \(\beta_s \propto \left( e^{-E_a/kT} + e^{-2(E_a+E_s)/kT} \right) \theta_e^2 \). The upper bound on \(\beta_s\) is derived using the above dependence from the lower bound \(= \Gamma(T_1)\). \(E_a=0.97 \text{eV}, E_s\) is set equal to a value that gives the largest increase). The parameter \(t\) is then evaluated using \(t = \beta_s a L_n\). This gives upper and lower bounds on \(t\): \(t_{u,l} = \frac{\Gamma(T_1)}{a^2 \lambda^2 r(T_2)} \left( 1, \left(\frac{1-\theta_e(T_1)}{r(T_2)}\right) \left( e^{-E_a/T_2} + e^{-2(E_a+E_s)/T_2} \right) \theta_e(T_1) \right)^2 \). - where \(T_2^+ (T_2^-)\) corresponds to the highest (lowest) temperature in the range of interest. The values of \(r(T_2^+)\) and \(r(T_2^-)\) are obtained from the data of Latyshev et al \([11]\) using \(E_b=4.34 \text{eV}, \Gamma(T_1)\) from a previous measurement of Bartelt et al \([34]\), \(E_a=0.97 \text{eV}, \theta_e(T_1)=0.1\) (measured by Yang et al \([31]\) and \(\theta(T_2^-)=0.167\) (as assumed previously). This results in \(7.7 \times 10^2 \mu m \leq t \leq 7.7 \times 10^3 \mu m \times 10^{3.1}\). The range of \(t\) therefore depends on the value of \(\lambda\).

The value of the parameter \(w\) used here is equal to the average terrace width in the experiment of Williams et al \([12]\) (=0.15 \(\mu m\)) who determine \(\rho_{eff}\) to be 0.20±0.03. It must be noted that the extraction of \(\rho\) from the experiment had used a theory \([35]\) which makes \(\rho_{eff} = \rho(w\lambda^{-1}=0)\) (\(w\) was much smaller than the average terrace width since in the theory used it corresponded to the distance between bunched steps). In this study it is assumed that \(\rho_{eff} = \rho(w\lambda^{-1}  0)\) - this may be a reasonable approximation since here \(\lambda_{min} =0.5 \mu m\) and the \(W_{max}\) in the experimental data used to determine \(\rho_{eff}\) was as large as 0.6 \(\mu m\). This approximation is motivated by the need to study the solution of \(\tau^{-1} = 0\) including the full non-linearity in \(w\lambda^{-1}\).

The procedure for determining \(E_s^u\) and \(F_\ell\) assumes that an electromigration force \(F\) causes the step bunching instability (\(\rho=0.2\)) with \(-F\) restoring the stability (\(\rho \geq 1\)). This assumption is motivated by the observation \([12]\) that a current in the step up direction
causes the step bunching whereas an equal magnitude in the step down direction results in uniformly spaced steps. $E_s^u$ & $F_\ell$ are determined by studying the solutions to $\tau^{-1} = 0$ (fixing $t, \lambda$ and $w$) for $\rho=0.2$ and $\rho=1.0$. The variation of $\tau^{-1}$ with $F$ (with typical values of $t, \lambda, w, E_s$ & $\rho$) is shown schematically in inset (a) of Fig. 4. Of interest is the solution that exists even in the limit $w\lambda^{-1} = 0$ (the other two solutions do not exist in this limit). The variation of this solution with $E_s$ (fixed $t, \lambda$ and $w$) for $\rho=0.2$ and $\rho=1.0$ is shown schematically in inset (b) of Fig. 4. The two curves show that beyond a certain value of $E_s$ a force $-F$ (with $F$ resulting in $\rho=0.2$) cannot restore stability. This value is therefore the upper bound ($E_s^u$) on $E_s$. Below $E_s^u$ the magnitude of $F$ needed for $\rho=0.2$ is larger. The value of $F$ at $E_s^u$ is therefore the lower bound ($F_\ell$) on $F$. $0 = F(E_s = 0, \rho = 0.2)$.

Fig. 4 shows the variation of $F_\ell$, $E_s^u$ and $F_0$ with the parameters $t$ and $\lambda$ $(w = 0.15 \mu m)$. As noted previously the range of the $t$ depends on the value of $\lambda$, with additional restrictions on the upper bound of $t$. These restrictions are due to the absence of the solution (of interest) to $\tau^{-1} = 0$ for small $\lambda$ and large $t$. This seems to correspond the behavior observed at higher temperatures [12] wherein a current in the step down direction causes the step bunching instability. For $tw \leq 1$, the curves in Fig. 4 correspond to the limit $w\lambda^{-1} \rightarrow 0$ and can be obtained by solving $\tau^{-1} = 0$ to zeroth order in $w\lambda^{-1}$. This gives

$$F = \frac{k_B T}{\lambda^2 t} \left( \frac{(1 + e^{-2E_s/k_B T}) - \rho(1 + e^{2E_s/k_B T})}{\rho - 1} \right) \tag{3}$$

Using the above expression, $E_s^u$, $F_\ell$ and $F_0$ are found to be

$$E_s^u = \frac{k_B T}{2} \ln \left( \frac{3 + \rho_0}{3\rho_0 + 1} \right) \tag{4}$$

$$F_\ell = \frac{k_B T}{\lambda^2 t} \left( \frac{4(1 - \rho_0^2)}{(3 + \rho_0)(3\rho_0 + 1)} \right) \tag{5}$$

$$F_0 = \frac{k_B T}{\lambda^2 t} \left( \frac{2(1 - \rho_0)}{1 + \rho_0} \right) \tag{6}$$

with $\rho_0 = 0.2$ (here). Equation 4 gives $E_s^u=0.05$ eV for the experiment of Williams et al [12]. This is much smaller than the barrier calculated here for the [211] step (0.61±0.07 eV)
suggesting that \([\overline{1}12]\) steps were seen in the experiment. From equn. 6 and the electric field in the experiment \([12]\) (700 V/m) the (maximum) charge needed on the adatoms (in units of the (negative) electronic charge) is estimated to be reasonably small- in the range \(3 \times 10^{-2}\) to \(3 \times 10^{-5}\). From Fig. 4 it can be seen that with a Schwoebel barrier the charge needed is always smaller than with a zero barrier. For \(tw > 1\), the deviation of the curves from the above expressions is significant - this is due to the dependence of \(\tau^{-1}\) on \(w\lambda^{-1}\) which require that terms of order \(w\lambda^{-1}\) and higher be considered. In this range, the minimum charge needed on the adatoms (using \(F_{\ell}\)) continues to have a reasonable lower limit as it is in the range \(2 \times 10^{1}\) to \(7 \times 10^{-5}\).

IV. CONCLUSIONS

In summary the adatom potential energy contours have been calculated for the 1×1 reconstructed Si(111) surface and the two high symmetry single height steps on it using the empirical Stillinger-Weber potential. From these plots diffusion barriers along the path of minimum barrier height can be calculated for transitions between any two minima. The results show that barriers for diffusion in the trench along the step edge are smaller than that between that global minima on the free surface. There is also a strong correlation between that adatom potential energy and the potential energy derived from the local geometry of atoms on the adatom free surface or surface or Si(111) surface (0.97±0.07 eV) and the Schwoebel barrier on the \([\overline{1}11]\) step (0.61±0.07 eV) are robust features due to changes in adatom coordination number. Interpreting recent electromigration experiments in the presence of a Schwoebel barrier shows that smaller values of electronic charge on the adatoms can account for the observations. It also suggests, in the limit where the diffusion length (\(\lambda\)) is much larger than the terrace width (\(w\)), that \([\overline{1}12]\) steps were observed in the experiment \([12]\). However, this conclusion relies on assumptions regarding the nature of the atomic processes at the step edge (that these processes may involve two atoms (at a kink site) which see the barriers as computed here) and that \(w\lambda^{-1} \to 0\). Future studies addressing
these assumptions may interpret electromigration experiments differently.

ACKNOWLEDGMENTS

One of the authors (S. Kodiyalam) wishes to thank E.D. Williams, N.C. Bartelt, Elain Fu, D.J. Liu, D. Kandel and S.V. Khare for useful discussions. This work has been supported by the NSF-MRG and the U.S. ONR.

APPENDIX A: ANALYSIS OF THE DIFFUSION EQUATION FOR STEP MOTION

The diffusion equation for non-interacting adatoms subliming in the presence of an electromigration force $F$ perpendicular to the step edge and the absence of an external flux may be written in the “adiabatic approximation” (which neglects the time derivative of the density) as follows: [14,29]

$$\frac{d^2 n}{dx^2} - f \frac{dn}{dx} - \frac{n}{\lambda^2} = 0$$  (7)

where $n$ is the density of adatoms, $f = F/k_BT$, $\lambda$ is the diffusion length and the positive $x$ axis coincides with the step down direction. This equation can be solved using the boundary conditions on the current $j (=D \left(-\frac{dn}{dx} + fn\right)$, where $D$ is the diffusion constant). These conditions determine the step velocity $V$ ($=a^2(-j_l + j_u)$, where $a^2$ is the inverse terrace density, $j_u$ is the current towards the step edge from the upper terrace and $j_l$ is the current away from the step edge on the lower terrace) and define the step kinetic coefficient $\beta$. In the presence of a Schwoebel barrier ($E_s$), this parameter is modeled as assuming the values $\beta_0$ and $\beta_1$ at the upper ($x = 0$) and lower ($x = W$) terrace step edges respectively, with $\frac{\beta_0}{\beta_1} = e^\epsilon$, where $\epsilon = \frac{2E_s}{k_BT}$. The boundary conditions can now be written as follows:

$$\left[-\frac{dn}{dx} + fn\right]_{x=0} = -\frac{te^\epsilon}{1 + e^\epsilon}(n(0) - n_e), \quad \left[-\frac{dn}{dx} + fn\right]_{x=W} = \frac{t}{1 + e^\epsilon}(n(W) - n_e)$$  (8)
where \( n_e \) is the equilibrium density and \( t = \frac{2 \beta_0 + \beta_1}{\alpha^2 D n_e} \). The solution to the diffusion equation under the above boundary conditions is shown below:

\[
n(x) = n_e (A e^{W \lambda^{-1} \eta_+} + B e^{W \lambda^{-1} \eta_-}) \tag{9}
\]

with

\[
\eta_{\pm} = f \lambda/2 \pm \sqrt{(1 + (f \lambda/2)^2)},
A = \frac{\phi \psi e^{W \lambda^{-1} \eta_+ - \varphi}}{\phi \psi e^{W \lambda^{-1} \eta_+ - \varphi} \chi e^{W \lambda^{-1} \eta_-}},
B = \frac{\phi - \chi e^{W \lambda^{-1} \eta_+}}{\phi \psi e^{W \lambda^{-1} \eta_+ - \varphi} \chi e^{W \lambda^{-1} \eta_-}}.
\]

The solution to the diffusion equation under the above boundary conditions is shown below:

\[
n(x) = n_e (A e^{W \lambda^{-1} \eta_+} + B e^{W \lambda^{-1} \eta_-}) \tag{9}
\]

with

\[
\eta_{\pm} = f \lambda/2 \pm \sqrt{(1 + (f \lambda/2)^2)},
A = \frac{\phi \psi e^{W \lambda^{-1} \eta_+ - \varphi}}{\phi \psi e^{W \lambda^{-1} \eta_+ - \varphi} \chi e^{W \lambda^{-1} \eta_-}},
B = \frac{\phi - \chi e^{W \lambda^{-1} \eta_+}}{\phi \psi e^{W \lambda^{-1} \eta_+ - \varphi} \chi e^{W \lambda^{-1} \eta_-}}.
\]

The velocity \((V_n)\) of a particular step edge \((X_n)\) can now be calculated:

\[
V_n = a^2 (-j_l(= j(x = 0, W = X_{n+1} - X_n)) + j_u(= j(x = W, W = X_n - X_{n-1}))
\]

From the functional form of the density and using \( D = \frac{A^2}{\tau f} \) (\( \tau f \) is the lifetime of an adatom) it may be seen that

\[
V_n = \frac{n_e a^2}{\tau f} \lambda (g_- + g_+) \tag{10}
\]

where \( g_{\pm} \) are dimensionless functions of dimensionless arguments given by:

\[
g_-(\epsilon, t\lambda, f\lambda, W \lambda^{-1}) = t\lambda \left[ e^{\frac{A+B-1}{2(1+e^\epsilon)}} \right],
g_+(\epsilon, t\lambda, f\lambda, W \lambda^{-1}) = t\lambda \left[ e^{\frac{A+B+1}{2(1+e^\epsilon)}} \right].
\]

with the symmetry \( g_+(-a, b, -c, d) = g_-(a, b, c, d) \).

**APPENDIX B: AN ATOMIC MODEL FOR THE STEP KINETIC COEFFICIENT**

The step kinetic coefficient \( \beta \) was introduced by Chernov [36] through the supposition that the currents \((j_l\) from the lower terrace and \(j_u\) from the upper terrace) towards a step edge (at \( x = X \)) are proportional to the deviation of the adatom density \( n \) in the neighborhood of the step from the equilibrium density \( n_e \). From the model adopted here it will be shown that in the presence of a Schwoebel barrier this parameter assumes different values \( i.e. \beta_0 \) and \( \beta_1 \) determining \( j_l \) and \( j_u \) respectively:

\[
\dot{j}_l = -\frac{\beta_0}{a^2} \left[ \frac{\theta(X^+ - \theta_e)}{\theta_e} \right], \quad \dot{j}_u = \frac{\beta_1}{a^2} \left[ \frac{\theta(X^- - \theta_e)}{\theta_e} \right] \tag{11}
\]
where \( a^2 = 1/(\text{terrace density}), \theta = na^2 \) and \( \theta_e = n_e a^2 \) with the positive \( x \) axis in the step down direction. These equations serve as the boundary conditions used in this work (eqn 8).

The temperature dependence of \( \beta_0 (\beta_1) \) can be derived assuming an activated model for adatom attachment-detachment at the step edge from the lower (upper) terrace with the single atom activation barrier being \( E_a (E_a + E_s) \) where \( E_a \) is the barrier on the free surface and \( E_s \) is the Schwoebel barrier. However, since silicon has two atoms in its unit cell, successful attachment-detachment processes at the kink sites of steps must involve two atoms. Single atom processes from energetically favorable step edge configurations lead to unfavorable ones and are expected to have very large barriers. Further, the probability of simultaneous attachment (detachment) of two atoms is proportional to \( \theta_e^2 ((1 - \theta_e)^2) \). The currents are therefore given by:

\[
\begin{align*}
  j_l &= -\nu_l e^{-\frac{2E_a}{k_B T}} a^2 (1 - \theta)^2, \\
  j_u &= \nu_u e^{-\frac{2(E_a + E_s)}{k_B T}} a^2 (1 - \theta)^2 \\
where a \parallel is the lattice constant along the step and \( \nu_{l,u} \) are “effective” attachment attempt frequencies. The vanishing of these currents in equilibrium (when \( \theta = \theta_e \)) determine the constants \( c_{l,u} \). Further assuming \( \nu_l = \nu_u = \nu \) and neglecting terms of the order \( (\theta - \theta_e)^2 \) gives:
\[
\begin{align*}
  j_l &= -\frac{2\nu\theta_e e^{-\frac{2E_a}{k_B T}}}{a \parallel (1 - \theta_e)} (\theta - \theta_e), \\
  j_u &= \frac{2\nu\theta_e e^{-\frac{2(E_a + E_s)}{k_B T}}}{a \parallel (1 - \theta_e)} (\theta - \theta_e)
\end{align*}
\]
from which \( \beta_0 \) and \( \beta_1 \) can be identified. Hence

\[
\begin{align}
\beta_0 + \beta_1 &= \frac{2\nu a^2}{a \parallel} \left[ \frac{\theta_e^2}{1 - \theta_e} \right] \left( e^{-\frac{2E_a}{k_B T}} + e^{-\frac{2(E_a + E_s)}{k_B T}} \right) \\
\frac{\beta_0}{\beta_1} &= e^{-\frac{2E_a}{k_B T}}
\end{align}
\]
To relate the step mobility $\Gamma$ and the step kinetic coefficient $\beta_s = \beta_0 + \beta_1$, the expression for the step velocity ($\frac{dX}{dt} = a^2(j_u - j_l)$) must be obtained in terms of $\beta_s$. From Chernov’s defining equations (11):

$$\frac{dX}{dt} = \frac{1}{\theta_e} (\beta_1 \theta(X^+) + \beta_0 \theta(X_-) - \beta_s \theta_e)$$  \hspace{1cm} (14)

This equation needs to be extended to account for the two dimensional character of the step: The currents towards the step edge are proportional to the deviation of the chemical potential $\mu$ from the equilibrium chemical potential near the step edge $\mu^*_e$. These relationships may be assumed to be the defining equations for the step mobilities $\Gamma_1$ and $\Gamma_0$:

$$j_u = \Gamma_0 \frac{a^2}{\theta_e^2} (\mu(X^-) - \mu_e^*), \quad j_l = -\Gamma_1 \frac{a^2}{\theta_e^2} (\mu(X^+) - \mu_e^*)$$  \hspace{1cm} (15)

Assuming the existence of a coarse-grained free energy functional $F$ of the step configuration $\{x(y)\}$, $\mu_e^*$ is given by Mullins [43] to be:

$$\mu_e^* = \mu_e + \frac{a^2}{k_b T} \frac{\delta F(x(y))}{\delta x}$$  \hspace{1cm} (16)

where $\mu_e$ is the equilibrium chemical potential on the terrace far away from the step edge. Further adopting his model of a dissolving substance for the adatoms, and in an approximation in which the deviation of the density $\theta$ from the equilibrium density $\theta_e$ (the density far away from the step edge) is much smaller than $\theta_e$, the chemical potential and the density can be related by [43]:

$$\mu(\theta) - \mu_e = k_b T \frac{\theta - \theta_e}{\theta_e}$$  \hspace{1cm} (17)

Using equations 16 and 17 it can be seen that the equilibrium density beside the step edge is different from $\theta_e$. [40–42] Further using equation 15, the step velocity can be given by:

$$\frac{\partial x}{\partial t} = \frac{1}{\theta_e} \left( \frac{\Gamma_1}{a^2} \theta(x^+) + \frac{\Gamma_0}{a^2} \theta(x^-) - \frac{\Gamma \theta_e}{a^2} \left(1 + \frac{a^2}{k_b T} \frac{\delta F(x(y))}{\delta x}\right) \right)$$  \hspace{1cm} (18)
where $\Gamma = \Gamma_0 + \Gamma_1$. In the absence of an external force on the adatoms and when attachment-detachment of atoms from the terrace onto the step edge is rate limiting in relation to terrace diffusion it is expected that $\theta(x^+) = \theta(x^-) = \theta_e$. Then, equation 18 reduces to the Langevin equation (without the noise term $\zeta$) [39,34]:

$$\frac{\partial x}{\partial t} = -\frac{\Gamma}{k_b T} \frac{\delta F(x(y))}{\delta x} + \zeta(y, t)$$

Within the small slope approximation ($\frac{\partial x}{\partial y} \ll 1$), $\frac{\delta F(x(y))}{\delta x} \propto \frac{\partial^2 x}{\partial y^2}$. The spatial average (over $y$, denoted by $<>$) of this term vanishes due to periodic boundary conditions. Identifying $<> x$ with $X$, assuming that the density is independent of $y$ and approximating $< \theta(x) >= \theta(X)$, equation 18 (on spatial averaging) gives:

$$\frac{dX}{dt} = \frac{1}{\theta_e} \left( \frac{\Gamma_1}{a^2} \theta(X^+) + \frac{\Gamma_0}{a^2} \theta(X^-) - \frac{\Gamma \theta_e}{a^2} \right)$$

Equations 14 and 19 agree if

$$\beta_{0,1} = \frac{\Gamma_{0,1}}{a^2} \Rightarrow \beta_s = \frac{\Gamma}{a^2}$$
REFERENCES

[1] R.L. Schwoebel and E.J. Shipsey, J. Appl. Phys 37, 3682 (1966)

[2] J.Villain, J. Phys. I 1, 19 (1991)

[3] M.D. Johnson, C. Orme, A.W. Hunt, D. Graff, J. Sudijono, L.M. Sander and B.G. Orr, Phys. Rev. Lett. 72, 116 (1994)

[4] M. Siegert and M. Plischke, Phys. Rev. Lett. 73, 1517 (1994)

[5] A.W. Hunt, C. Orme, D.R.M. Williams, B.G. Orr and L.M. Sander, Europhys. Lett. 27, 611 (1994)

[6] I. Elkinani and J. Villain, J. Phys. I (France) 4, 949 (1994)

[7] C.J. Lanczycki and S. Das Sarma, Univ. of Maryland preprint (1995)

[8] J. Chevrier, A. Cruz, N.Pinto, I.Brebezier and J. Derrien, J. Phys. I (France) 4, 1309 (1994)

[9] H.N. Yang, G.C. Wang and T.M. Lu, Phys. Rev. B 51, 14293 (1995)

[10] C.J. Lanczycki, Y.N. Yang, E. Fu, R. Kotlyar, E.D. Williams and S. Das Sarma, Univ. of Maryland preprint (1995) (1995) “Dynamical Scaling and Phase Separation in Kinetic Growth Models with

[11] A.V. Latyshev, A.L. Aseev, A.B. Krasilnikov and S.I. Stenin, Surf. Sci. 213, 157 (1989)

[12] E.D. Williams, E. Fu, Y.N. Yang, D. Kandel and J.D. Weeks, Submitted to Surf. Sci.

[13] F.H. Stillinger and T.A. Weber, Phys. Rev. B 31, 5262 (1985)

[14] S.S. Stoyanov, H. Nakahara and M. Ichikawa, Jpn. J. Appl. Phys. 33, 254 (1993)

[15] T.W. Poon, S. Yip, P.S. Ho and F.F. Abraham, Phys. Rev. Lett. 65, 2161 (1990)

[16] X.P. Li, P.B. Allen and J.Q. Broughton, Phys. Rev. B 38 3331 (1988)
[17] D.J. Chadi and J.R. Chelikovsky, Phys. Rev. B 24, 4892 (1981)

[18] C. Roland and G.H. Gilmer, Phys. Rev. Lett. 67, 3188 (1991)

[19] C. Roland and G.H. Gilmer, Phys. Rev. B 46, 13428 (1992)

[20] C. Roland and G.H. Gilmer, Phys. Rev. B 46, 13437 (1992)

[21] S. Kodiyalam, K.E. Khor, N.C. Bartelt, E.D. Williams and S. Das Sarma, Phys. Rev. B 51, 5200 (1995)

[22] K.E. Khor and S. Das Sarma, Chem. Phys. Lett. 134, 43 (1987)

[23] J.E. Northrup and M.L. Cohen, Phys. Rev. B 29, 1966 (1984)

[24] J.E. Northrup, Phys. Rev. Lett. 57, 154 (1986)

[25] K.E. Khor and S. Das Sarma, Phys. Rev. B 39, 1188 (1989)

[26] K.E. Khor and S. Das Sarma, Phys. Rev. B 36, 7733 (1987)

[27] M.T. Yin and M.L. Cohen, Phys. Rev. B 26, 5668 (1982)

[28] P. Bennema and G.H. Gilmer, in: Crystal Growth: an introduction., Ed. P. Hartman (American Elsevier Publishing Company, N.Y., 1973)

[29] R. Ghez, H.G. Cohen and J.B. Keller, Appl. Phys. Lett. 56, 1977 (1990)

[30] W.K. Burton, N. Cabrera and F.C. Frank, Phil. Trans. Roy. Soc. (London) 243A, 299 (1951)

[31] Y.N. Yang and E.D. Williams, Phys. Rev. Lett. 72, 1862 (1994)

[32] E. Fu, private communications

[33] R.D. Meade and D. Vanderbilt, Phys. Rev. B 40, 3905 (1989)

[34] N.C. Bartelt, J.L. Goldburg, T.L. Einstein, E.D. Williams, J.C. Heyraud and J.J. Métois, Phys. Rev. B 48, 15453 (1993)
[35] D. Kandel and J.D. Weeks, Phys. Rev. Lett. 74, 3632 (1995)

[36] A.A. Chernov, Sov. Phys. Usp. 4, 116 (1961)

[37] E.D. Williams, private communications

[38] N.C. Bartelt, private communications

[39] N.C. Bartelt, J.L. Goldburg, T.L. Einstein and E.D. Williams, Surf. Sci. 273, 252 (1992)

[40] N.C. Bartelt, T.L. Einstein and E.D. Williams, Surf. Sci. 312, 411 (1994)

[41] M. Uwaha and Y. Saito, Phys. Rev. B 68, 224 (1992)

[42] G.S. Bales and A. Zangwill, Phys. Rev. B 41, 5500 (1990)

[43] W.W. Mullins, in Metal surfaces, Eds. W.D. Robertson and N.A. Gjostein (American Society for Metals, Metals Park, OH, 1963) p. 17
FIGURES

FIG. 1. One bilayer of the Si(111) surface consisting of the upper monolayer (grey) and lower monolayer (black). The figure shows the threefold and reflection symmetry of this surface: Steps running along directions with equal $\theta$ are identical. (Borrowed from reference [21])

FIG. 2. The Si(111) surface (a) (the upper monolayer is shown in grey and the lower monolayer in black), the $[\overline{2}11]$ step (d) and the $[\overline{1}12]$ step (g) (for the step configurations the upper bilayer is shown with larger atoms as compared to the lower bilayer). (b), (e) & (h) show the corresponding adatom binding energy $V(x, y)$. (c), (f) & (i) show the corresponding binding energy derived from the local geometry $V_{lg}(x, y)$. Minima, saddle points and maxima are marked (labeled) by +(m), *(s) and $\times$(M) respectively with the figure in parenthesis being their corresponding value in eV. In (b) & (c) the contours are 0.1 eV apart. In (e), (f), (h) & (i) they are 0.2 eV apart. In (e) & (h) contours of $V \geq -2.2$ eV and in (f) & (i) those of $V_{lg} \geq -1.9$ eV are marked with dashed lines. The contour plots suggest a strong correlation between $V$ and $V_{lg}$. The diffusion barrier on the surface is determined by m1 & s1 in (b) & (c). The Schwoebel barrier is determined by s3 in (e) & (f) whereas it is determined by s5 in (h) and s6 in (i). There is a one-to-one correspondence between the barrier determining features in $V(x, y)$ and $V_{lg}(x, y)$ for the Si(111) surface and the $[\overline{2}11]$ step suggesting that the Schwoebel barrier on the $[\overline{2}11]$ step is robust feature.

FIG. 3. Plots of the adatom potential energy derived from the local geometry of fixed atoms $V_{lg}$ vs the actual adatom potential energy $V$. The straight line fits show the strong correlation between $V_{lg}$ and $V$. The rough configuration independence of the relationship suggests that it is a characteristic of the (111) surface.
FIG. 4. Inset (a) shows schematically the variation of $\tau^{-1} = k_+ - \rho k_-$ with $F$. The solution to $\tau^{-1} = 0$ (of interest) is $F_r$ which exists even in the limit $w\lambda^{-1} = 0$ whereas the other two do not. Inset (b) shows schematically the variation of $F_r$ with $E_s$ for $\rho = 1.0$ and $\rho = 0.2$. The upper bound on $E_s (E^u_s)$ is determined from the condition $F(E_s > E^u_s, \rho = 1.0) < -F(E_s > E^u_s, \rho = 0.2)$. It can be seen that $F(E^u_s, \rho = 0.2)$ is the lower bound on $F (F_\ell)$. $F_0 = F(E_s = 0, \rho = 0.2)$. For the curves shown, $w = 0.15\mu m$, $0.5\mu m \leq \lambda \leq 0.5 \times 10^3 \mu m$ (7 values equally spaced on the logarithmic scale) with the range of $t$ depending on $\lambda$: $\frac{7.7 \times 10^3}{\lambda^2} \leq t \leq \frac{7.7 \times 10^3}{\lambda^3} \times 10^{3.1}$ ($\lambda > 7\mu m$). The upper (lower) limits of $t$ are marked by + (×). For $\lambda < 7\mu m$ the upper limit of $t$ is forced to be smaller than that estimated since the solution $F_r$ ceases to exist. For $\lambda < 1 \mu m$, $F_r$ does not exist for even the smallest $t$. This shows that $\lambda_{\min} = 1 \mu m$. For $w\lambda^{-1} \to 0$, $E^u_s = 0.35k_B T = 0.05 \text{ eV}$ (for the experiment in ref. 5) - significantly lesser than that calculated here for the $\{\overline{1}12\}$ step (0.61±0.07 eV). This suggests that $[\overline{1}12]$ steps were observed.
Fig 1. “Calculated Schwoebel Barriers ……” by S. Kodyalam et al.
Fig 2a. “Calculated Schwoebel barriers ...” by S. Kodiylam et al.
Fig 2b. "Calculated Schwobel Barriers ......." by S. Kodiyalam et al
Fig 2c. “Calculated Schwobel Barriers .......” by S. Kodiyalam et al
Fig 2d. “Calculated Schwobel barriers ...” by S. Kodiyalam et al.
Fig 2e. “Calculated Schwoebel Barriers ……” by S. Kodiyalam et al
Fig 2f. “Calculated Schwoebel Barriers ……” by S. Kodiyalam et al
Fig 2g. “Calculated Schwoebel barriers ...” by S. Kodiyalam et al.
Fig 2h. “Calculated Schwoebel Barriers .......” by S. Kodiyalam et al
Fig 2i. “Calculated Schwoebel Barriers …..” by S. Kodiyalam et al
Fig 3. “Calculated Schwobel Barriers ……” by S. Kodyalam et al
Fig 4. “Calculated Schoebel Barriers .......” by S. Kodyalam et al.