Nonequilibrium influence of upward atomic mobility in one-dimensional molecular-beam epitaxy

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We have implemented barriers to thermally activated hopping in stochastic solid-on-solid growth simulations on one-dimensional substrates, emphasizing the extreme special cases of zero and infinite barriers to downward (i.e., towards the substrate) and upward (i.e., away from the substrate) diffusion for a range of temperatures. At a single temperature, we also introduced various finite, nonzero energy barriers to downward atomic hopping in order to systematically study nonequilibrium effects of a diffusion barrier. Our results indicate that within the solid-on-solid restriction generic growth stability is likely in molecular-beam epitaxy unless a sufficiently large diffusion barrier to downward hopping exists in concert with upward atomic mobility. Our results also demonstrate the difficulty of experimentally extracting dynamical growth exponents due to transient and crossover effects which dominate the kinetics of epitaxy.

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A clear and unified theoretical understanding of the physics of growing interfaces evolving under nonequilibrium kinetic growth conditions remains elusive despite the emergence of the dynamical scaling hypothesis and coarse-grained stochastic continuum equations as tools. It was postulated [1] that growing surfaces could be viewed as self-affine fractals with the property of statistical scale invariance. Root mean square surface height fluctuations, $w(t,L)$, therefore should show a power law dependence on the growth time (t) and lateral system size (L). Considerable work [2–8] has been devoted to developing generalized Langevin-type dynamical differential equations to describe the asymptotic growth characteristics. The simplest case had been pioneered by Edwards and Wilkinson (EW) [2], who studied growth under sedimentation by letting the randomly deposited atoms relax to local height minima. Several early numerical stochastic growth models verified their quantitative results [9–11], namely that $w(t,L) \sim t^{\beta}$ ($t << L^z$) and $w(t,L) \sim L^{\alpha}$ ($t >> L^z$) [where $w(t,L)$ is the surface width, $w(t,L) = \langle (h(\vec{x},t) - \overline{h(t)})^2 \rangle^{1/2}$, with $\overline{h(t)}$ being the average surface height and $\langle \cdots \rangle$ indicates both a spatial and a statistical average] with $\beta \approx 1/4(\log)$ and $\alpha \approx 1/2(\log)$ for $d' = 1(2)$ substrate dimension(s), and the dynamical exponent $z = \alpha/\beta$. The EW equation [Eq. (1) below] can be verified by Fourier transform methods to show this scaling behavior. The EW equation is

$$\frac{\partial h(\vec{x},t)}{\partial t} = \nu_2 \nabla^2 h(\vec{x},t) + \eta(\vec{x},t), \tag{1}$$

where $h(\vec{x},t)$ is the local dynamical height at substrate position $\vec{x}$ and η represents a random, uncorrelated white noise associated with the incident flux of particles. It has been shown that, in addition to the gravitational forces involved in sedimentation, desorption of atoms from growth fronts also leads to EW-type universality [7]. In general, the Laplacian term in the EW equation (with $\nu_2 > 0$) describes the smoothening of the growing surface due to surface tension forces, and is often present in dynamical growth. The case of $\nu_2 < 0$, i.e., a negative surface tension term, should, in general, lead to instability without any dynamic scaling behavior [7,12].

For a process like semiconductor crystal growth via molecular-beam epitaxy (MBE) where neither gravitation nor desorption is quantitatively important, it is not manifestly obvious that the EW paradigm applies. In MBE, surface diffusion in a strong chemical bonding environment is the dominant relaxation process. It is not the physics of sedimentation which describes the interface dynamics in MBE growth, but a general attraction of surface atoms towards a substrate where particles achieve a maximal number of bonds. This is viewed as a statistical migration towards the substrate, whereby atoms sample numerous surface sites, staying longest in locations with high coordination. In this paper, we use the term "downward" diffusion to mean interlayer atomic mobility towards the substrate whereas "upward" diffusion means interlayer atomic mobility away from the substrate and "lateral" diffusion implies intralayer atomic diffusion.

Dynamical growth [13] simulations involving diffusion toward tightly bonded surface kink and trapping sites in general do not agree with the simple EW results [3,4,6], although the issue is by no means clearly resolved yet [14,15]. While a scaling hypothesis remains valid in such kink-diffusion simulations, the growth exponents numerically obtained via $w(t,L)$ increase to $\beta_{eff} \approx 0.371$ and $\alpha_{eff} \approx 1.32$ [4] in $(1+1)$-dimensions. Rather than the second-order Eq. (1), these exponents are reasonably consistent with the fourth order equation

$$\frac{\partial h(\vec{x},t)}{\partial t} = -\nu_4 \nabla^2 (\nabla^2 h(\vec{x},t)) + \eta(\vec{x},t), \tag{2}$$

which has been rationalized as the lowest order expansion for surface diffusion driven by a local chemical po-

tential gradient [16]. Given the nonequilibrium nature of this problem, it is, however, not clear that we can invoke a chemical potential gradient which drives surface diffusion. Based on simulational evidence [3,6,17], one associates the $\nabla^2(\nabla^2 h)$ term with diffusion to sites of increased coordination. Crossover effects associated with these discrete dynamical growth simulation models [15,18] are not completely understood at the present time. It should be emphasized, however, that Eq. (2) and the associated kink-diffusion discrete dynamical simulations have recently been shown to exhibit anomalous dynamical scaling behavior, which is the subject of several recent publications [12,14,15,19,20]. While the anomalous dynamic scaling of the fourth-order linear differential equation, Eq. (2), itself is trivially understood [19,20], the nature of dynamic scaling in the corresponding discrete dynamical growth models [3,6,18] has remained unsettled and is currently a subject of vigorous theoretical activity [14,15,21].

Both Eqs. (1) and (2) describe conservative growth (i.e., the crystal volume equals the total volume of particles deposited so that no desorption occurs and no holes or overhangs exist), which in general must obey the equation $\frac{\partial h}{\partial t} = -\vec{\nabla} \cdot \vec{j} + \eta$, where $\vec{j}$ is the surface current of atoms. Actual MBE growth involves very few defects (as evidenced by layer-by-layer oscillations seen, for example, by reflection high-energy electron diffraction), leading to the extensive use of conservative solid-on-solid (SOS) growth models in its study. To the order of Eq. (2), an equation containing all linear and nonlinear conservative terms consistent with the symmetries of the problem reads as [4,5,22]

$$\frac{\partial h(\vec{x},t)}{\partial t} = \nu_2 \nabla^2 h(\vec{x},t) - \nu_4 \nabla^2(\nabla^2 h) + \lambda_{42}\nabla^2(\nabla h)^2 + \lambda_{43}\nabla(\nabla h)^3 + \eta(\vec{x},t). \quad (3)$$

The ν_2 (or EW) term, when present, always controls the asymptotic scaling behavior, and when $\nu_2 = 0$, the $\lambda_{43}(\nu_4)$ term is the most (least) relevant in a dynamical renormalization group sense [5]. No atomistic process leading specifically to the λ_{43} term has yet been identified, but the migration of atoms from kink sites (both upwards and downwards) in various models has been shown to produce the nonlinear term $\nabla^2(\nabla h)^2$ [5,7,17]. One expects [5,22] the λ_{43} term to show up as a higher order correction to the EW ν_2 term on dimensional grounds—this has recently been verified in some dynamical simulations [14,18]. For real MBE, many physical processes may be active at the microscopic level, and their collective effect on the scaling properties of surfaces is the motivation for our study. All our results are in the physically less relevant $1+1$ dimensions (i.e., $(d'=1)$-dimensional substrates) where large simulations can be carried out; the corresponding simulations in the realistic $(2+1)$ dimensions are computationally prohibitive at the present time.

Several groups have recently analyzed simulations using thermally activated atomic hopping [3,4,17], introducing new length ("diffusion length") and time scales ("hopping time") into the problem. Das Sarma and Tamborenea [3] looked at a model without upward hopping, finding an effective exponent which generally decreased with increasing temperature (or equivalently, increasing diffusion length) but showed a short plateau near $\beta = 3/8$ corresponding to the dynamic scaling implied by Eq. (2). They also give evidence [4] that the decrease in β at high temperatures is a finite size effect which obscures any EW-type universality which may be present at higher temperatures. In a similar model (but with upward hopping allowed), Wilby *et al.* [17] showed results at two temperatures: they observed the ν_4 term at both temperatures, but the nonlinear λ_{42} term became effective at very long times at the higher temperature. The observation of EW scaling in the former model was indirectly inferred [4] by analogy with a related dynamical model with an adjustable diffusion length, while a proper choice of T (to minimize finite time and/or size effects) resulted in the appearance of the λ_{42} term in the later. These stochastic MBE growth studies strikingly demonstrate the grave difficulties in extracting growth exponents from experimental MBE studies. Even in the simplest ideal MBE growth model, finite size and crossover effects are so intrinsically intertwined with the dynamical scaling behavior that it may be impossible to infer the true asymptotic growth exponents [23]. Indeed, the experimental observations of growth, while showing scaling in general, have not converged to any consensus about the values of the growth exponents, with β_{eff} varying from ~ 0.2 [24] all the way to ~ 1.0 [25], and α_{eff} has been measured from 0.47 ± 0.02 [26] to 0.79 ± 0.05 [27] [all in $(2+1)$-dimensional studies]. Herein, we will attempt to indicate why one might unavoidably observe various values of β_{eff} for real growth within a simple $(1+1)$-dimensional ideal stochastic MBE growth model where diffusion is driven by activated hopping.

Our growth simulations occur on a $(d=2)$-dimensional square lattice from a flat one-dimensional substrate, with a lateral substrate size $L = 4000$–10000 lattice sites. Particles land randomly on the surface at a rate of $R_{dep} = 1$ layer/sec, incrementing the height above a randomly selected substrate site by one unit. In addition, *any* surface atom may undergo a hopping event, modeled as a thermally activated process with a site dependent activation energy, $E_a(n)$, where $n = n(\vec{x},t)$ is the number of occupied nearest neighbors of the site at $\vec{x}$ at the time of hopping, t. We use an Arrhenius form for calculating the hopping rates: $R_n = \frac{k_B T}{h} \exp[-E_a(n)/k_B T]$. We take $E_a(n) = E_0 + E_b n$, where $E_0 = 1.0\,\text{eV}$ models a general affinity of atoms for the surface, and the bond energy $E_b = 0.3\,\text{eV}$. Atoms with $n = 1, 2$, or 3 may hop, provided that no deviations from an SOS crystal occur (i.e., voids, overhangs, defects are not allowed). Evaporation is neglected throughout. Note that the choice of activation energies automatically determines the interesting temperature window for the growth problem, and our parameters are chosen to be qualitatively consistent with semiconductor MBE growth.

Temperatures range from $T = 450$ K when $R_1 < R_{dep}$ to $T = 675$ K, where $R_1 >> R_{dep}$, $R_2 > R_{dep}$, and $R_3 \sim 0.1\,R_{dep}$. At $T \approx 510$ K $R_1 = R_{dep}$, thus our temperature range covers the whole crossover regime. The growth temperature, by determining the hopping

rates, controls the crossover time scale in an exponential manner—in particular, it is well known [3,4] that at the lowest temperatures, $T < 450\,\mathrm{K}$ in this work, $\beta_{eff} \approx 1/2$ corresponding to random deposition because the time scale for any activated diffusion to occur is exponentially long. The landing site of a hopping particle is chosen randomly from among the eligible nearest neighbor columns, with constraints on the change in height as noted below. If there is no final configuration dependence in the hopping rate, the Arrhenius form for the rates assures that the local detailed balance condition is obeyed.

Our Monte Carlo implementation allows a variable degree of coarseness in executing the hopping depending on how frequently searches for eligible atoms occur. This is accomplished by letting a fraction $\frac{1}{m_n}$ of the eligible, appropriately bonded particles to hop after $\frac{1}{R_n}\frac{1}{m_n}$ seconds. Being interested in the early transient behavior, we chose m_n to search for potential hops after every deposition event for $n = 1, 2$, and an order of magnitude (or more) less frequently for triply bonded atoms. To avoid systematic errors, adjustments in m_n were made with changes in L. This technique resulted in excellent resolution of the early time behavior over the full range of temperatures.

We have looked at four distinct SOS models with this method, abbreviated as UD, NU, ND, and LAT, distinguished by the set of allowed landing sites for diffusing atoms. Most generally, lateral (in-plane), upward and downward hops occurred (abbreviated as the UD model), with all energy barriers calculated using the same energy parameters E_0 and E_b as quoted above. The NU model imposes an infinite barrier to upward hopping, with in-plane and downward hopping being unaffected, while the unphysical ND model instead permits only upward and lateral hops, giving an infinite barrier to downward diffusion. Finally, we permit only lateral hops in the LAT model. The LAT and ND models are interesting only as extremes, being limiting cases of nonequilibrium growth including a diffusion barrier, whereby particles experience an extra additive barrier, E_s, to diffusing down at a step edge [28]. The size of the diffusion barrier is generally not known for semiconductors, but our ND and LAT models extremely overemphasize the effect. We point out that our UD model obeys the detailed balance condition whereas the other three models (i.e., NU, ND, and LAT) are manifestly nonequilibrium in that they violate the principle of detailed balance because the hopping is dependent upon the final configuration. Thus the UD model is really the only physically allowed model even though the NU model is also a reasonable description of MBE growth at temperatures which are not too high. There are ways [29] of incorporating a diffusion barrier in MBE growth simulations explicitly obeying the principle of detailed balance, but one must either relax the simplicity of a nearest-neighbor interaction model used in our work or introduce by hand a final-state dependence into the hopping rates in such a way as to restore detailed balance. Our interest in this paper being on a qualitative and fundamental understanding of the trends associated with various *nonequilibrium* effects, the simplistic modeling employed in the NU, ND, and LAT models is sensible provided we do not make explicit comparison with experimental results (except for the UD model).

To get a feel for how drastically temperature influences the surface morphology, we present in Fig. 1 the surface height profiles for $T = 500, 600$, and 650 K after growth times of 100, 500, and 2000 layers in the UD and NU models for $L = 4000$. Note the change in vertical scale used due to the large disparity in the surface width as the temperature changes, and that the average height has been shifted in each case for clarity. At $T = 500$ K [Figs. 1(a) and 1(b)], the up-hopping has no gross visible effect and the NU and UD models look very similar. One can see the very random, noiselike quality at $t = 100$ begin to look more correlated on this substrate length scale after 2000 layers, reflecting the slow rate of hopping. In both models, as T rises, the height fluctuations become more subdued, and one sees small scale structures at early times coalesce into large features as growth proceeds. The UD and NU models evolve differently with temperature once the hopping rate exceeds the deposition rate, and one observes a considerably smoother surface in the NU case at $T = 650$ K [Fig. 1(f)], with few of the large steps that are readily apparent at all temperatures and times in the UD model. We have not presented morphologies for the LAT or ND models, but in general they (the ND model especially) exhibit a more spiked appearance than even the $T = 500$ K cases shown here and are unphysically rough.

To study the scaling properties of these models, we monitored the surface width as a function of time, from which β_{eff} was extracted as the slope of a log-log plot of $w(t)$. Consider first the UD model, where up- and down-hopping occur. At very early times and at all temperatures random, uncorrelated growth with $\beta_{eff} = 1/2$ was seen while at late times ($\sim$ 2000 layers) β_{eff} has decreased to ≈ 0.35 with a slight temperature dependence, shown as triangles in Fig. 2(a). Interestingly, the change in β_{eff} with time did not occur monotonically: before attaining the long time value, an intermediate time regime ($\sim$ 1–20 layers) occurred for $T \geq 550\,\mathrm{K}$ with a lower value of β_{eff} and a more pronounced temperature dependence. Because we permit hopping continuously in our simulation, this slope can be measured accurately.

The more frequently studied situation corresponds to the NU model, with all diffusion being either downward or parallel to the original substrate. The β_{eff} versus T plot [Fig. 2(b)] shows deviations from the UD model of Fig. 2(a) for $T \geq 550\,\mathrm{K}$ [$R_1 \approx 14R_{dep}$ and $R_2 \approx (1/40)R_{dep}$]. Instead of a large plateau at $\beta_{eff} \approx 0.35$, the exponent now displays a clear decreasing trend with no indications of a plateau. For all values of T (and all times), $\beta_{eff}^{\mathrm{NU}} \leq \beta_{eff}^{\mathrm{UD}}$, in keeping with our intuition that up-hopping should lead to relatively more roughened growth. We emphasize that the unrestricted, strong upward hopping in the UD model has not made the growing surface unstable, however, and β_{eff} never exceeds 0.5.

In both the UD and NU models for temperatures where the hopping rate R_1 is comparable to or greater than the deposition rate, β_{eff} initially falls below its asymp-

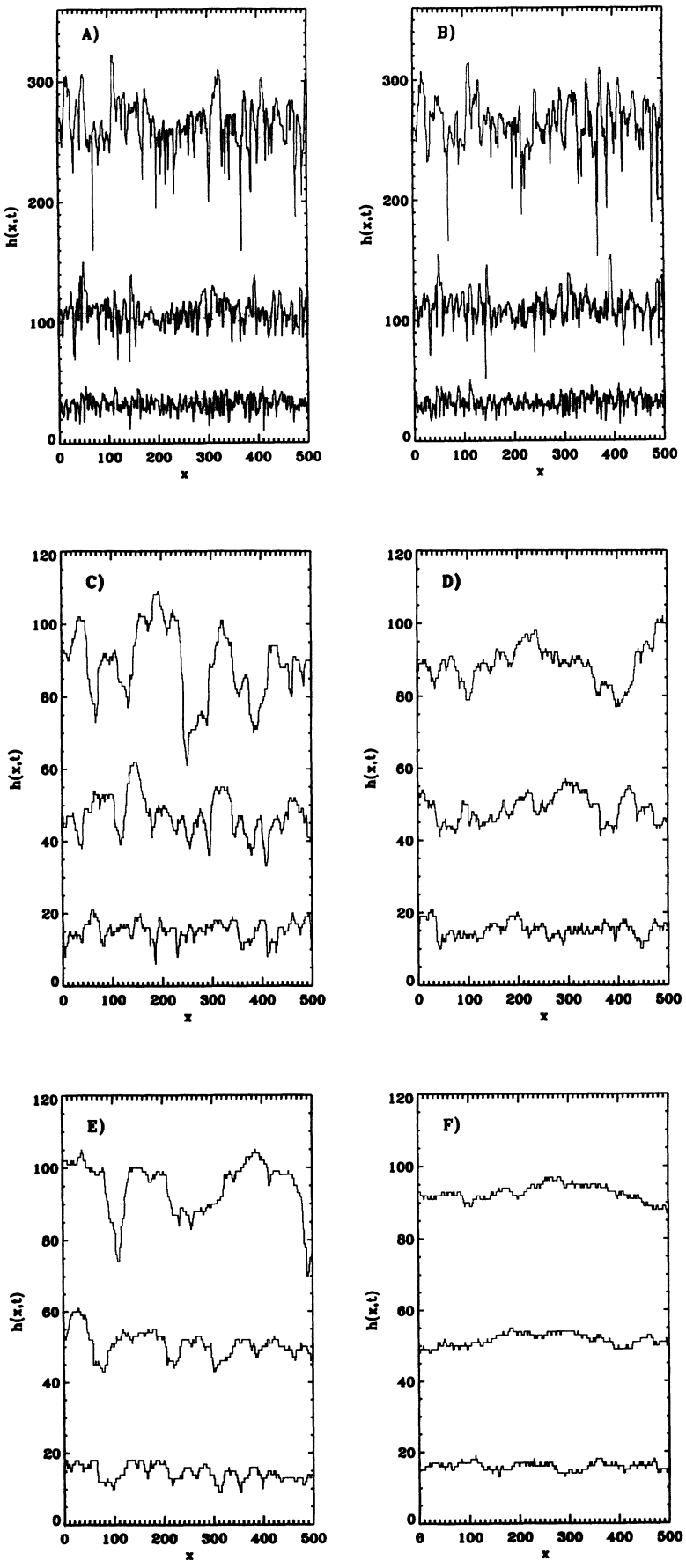

FIG. 1. Morphologies for $t = 100, 500$, and 2000 layers in the UD and NU models for a system size of $L = 4000$ at $T = 500$ K [(a) and (b)], $T = 600$ K [(c) and (d)], and $T = 650$ K [(e) and (f)]. Figures (a), (c), and (e) are snapshots of the UD model, and the NU model is shown in Figs. (b), (d), and (f).

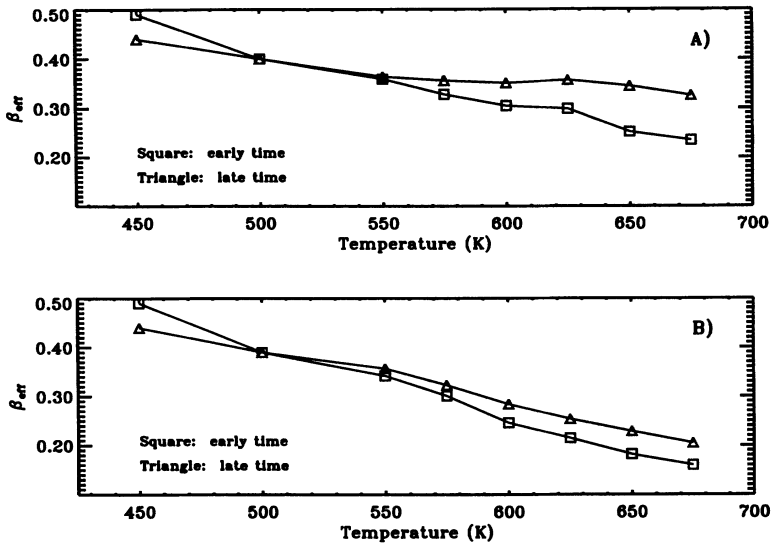

FIG. 2. Effective growth exponent, β_{eff}, versus temperature T [□: early time exponents (up to roughly 20 layers); △: late time exponents (more than about 50–100 layers)]. All runs have $L = 4000$ except for $T = 675$ K, where $L = 10\,000$. We have averaged over 3–10 runs. (a) UD model. (b) NU model.

totic value (β^a_{eff}, measured at the latest accessible times $t > 100$) early in the growth (β^e_{eff}, measured for $t \leq 20$ layers) so that $\beta^e_{eff} < \beta^a_{eff}$. It is, in principle, possible for β^a_{eff} to be somewhat lowered by saturation effects which have not yet manifestly appeared, but we have taken care to avoid such effects. The early exponent β^e_{eff} is obviously affected by finite time effects. When up-hopping occurs, the difference in these values, $\Delta\beta \equiv (\beta^a_{eff} - \beta^e_{eff})$, increases with temperature, whereas forbidding up-hops leads to a smaller, positive $\Delta\beta$ that seems to saturate beyond $T \approx 600$ K. The physical process causing the initially small value of the slope thus appears to be general, occurring in any stable model possessing thermally activated hopping, and not an artifact of strong upward mobility. Upward hopping enhances the difference in β_{eff} between the early and late growth, but is not essential to the existence of that difference.

Why should there be a positive $\Delta\beta$, rather than a simple monotonic crossover to β^a_{eff} from the $\beta_{eff} = 1/2$ random regime? In most previous numerical studies of conservative dynamical growth models [1,3,6,9,10], this transition indeed appears monotonic: in finite-T Monte Carlo simulations or stochastic models where variable diffusion lengths are permitted as a function of temperature a positive $\Delta\beta$ emerges [3,4,17]. Nonmonotonic β_{eff} is also fairly common in the ballistic deposition and Eden models which belong to the Kardar-Parisi-Zhang universality [8] and are manifestly non-SOS in nature [30,31]. We know of a only single instance within a *dynamical* SOS model where a nonmonotonic β_{eff} can be seen ([31], see Fig. 3 therein), where increasing the diffusion length leads to layer-by-layer growth oscillations and consequently a nonmonotonic β_{eff}.

Therefore, this initial drop in slope appears to result from the introduction of a new length scale in the problem, namely the diffusion length l [23], measuring the distance a surface particle can travel before its eventual incorporation into the bulk. Since the surface starts out flat, at early times incident particles (typically with only a single bond) initially can explore long distances before encountering highly coordinated sites required for their incorporation. At later times the growing surface is kinetically rough providing numerous nearby "active" sites where the freshly incident atoms may become incorporated, so that all surface diffusion takes place over shorter length scales. Consequently, for $T \geq 550$ K, as height fluctuations on the order of unity begin to develop after a certain time ($t \sim 20$ layers, on average) the incident particles are incorporated into the growing film within a shortened distance and β_{eff} experiences an increase over β^e_{eff}. Thus the diffusion length becomes a dynamical function of the evolving surface morphology. We believe that the finite value of $\Delta\beta$ is a direct manifestation of layer-by-layer growth oscillations attempting to emerge at the early stages of MBE in this parameter range. In general, layer-by-layer growth oscillations are more pronounced in (2 + 1)-dimensional stochastic simulations [32] than in one-dimensional MBE growth.

An interesting difference in β^a_{eff} between the NU and UD models is that the UD model produces a much more stable value (near ≈ 0.35) over a broad range of temperature where R_1/R_{dep} goes from ≈ 0.8 to ≈ 2700, whereas β^a_{eff} drops from ≈ 0.39 to ≈ 0.20 over the same temperature range in the NU model. That an overemphasis of the destabilizing effect of upward hopping (which in real MBE growth may be rare) should yield a nearly unchanging β^a_{eff} is curious. But in light of the fact that our simulation allows a particle to diffuse to reach a nearby energy minima, where hopping rates are exponentially lower, it is reasonable that $\beta^a_{eff} \approx 3/8$ for the UD model, corresponding to Eq. (2). Previous stochastic simulations [3,4,17] using only downward and lateral diffusion to energy minima also show this slope. In this sense, surprisingly, up-hopping does not seem to alter the physics embodied in Eq. (2), and actually it may better manifest such behavior by minimizing the obscuring effects of the long diffusion length which may be causing the high temperature decrease of β^a_{eff} in the NU case. We should mention, however, that our measured $\beta_{eff} \approx 0.35$ for the UD model is consistent (within numerical errors)

with the nonlinear Lai–Das Sarma–Villain (LDV) equation [Eq. (3) with $\nu_2 = \lambda_{43} = 0$] which in $1+1$ dimensions has $\beta = 1/3$ [5]. A dynamical simulation [5] which manifested this universality class allowed doubly bonded atoms to hop up or down provided that the number of bonds did not decrease: our stochastic models also include such processes, and there is always the possibility that some nonlinear effects may be present in our models particularly because the nonlinear $\nabla^2(\nabla h)^2$ term is more relevant in a renormalization group sense than the linear $\nabla^4 h$ term. Without measuring some other growth exponent, we cannot distinguish between the linear and nonlinear fourth order equations just based on our measurement of $\beta_{eff}^{UD} = 0.35$.

To make any identification with a continuum equation, an estimate of α, for example, is needed. Typical methods for obtaining α_{eff} are to plot the saturation width versus system size or to study the short distance behavior of the surface height-height correlation function (for anomalous dynamical scaling these two studies produce different exponents because the local and global scaling behaviors are different [14,15]). Here we have monitored the mean square surface gradient, $G(t,L) \equiv \langle(\nabla h)^2\rangle = \langle(h(x+1,t) - h(x,t))^2\rangle$ where the average is over the substrate coordinate x. Within the standard dynamic scaling hypothesis [1], for any universality class with $\alpha < 1$, which for (1+1)-dimensional SOS models corresponds only to the EW case ($\alpha = 1/2$) or the less relevant $\lambda_{43} \neq 0$ situation ($\alpha = 3/4$), the quantity G will quickly saturate to a constant. This behavior is differentiated from the cases of $\alpha = 1$ (λ_{42} term is the most relevant) where $G \sim \log(t)$, and $\alpha = 1.5$ [Eq. (2)] for which $G \sim t^{1/4}$ [33]. The quantity G manifests power law time dependence in all models (both discrete and continuous) showing anomalous dynamic scaling whereas in the usual dynamic scaling, where local and global scaling behaviors are not differentiated, $G(t)$ typically saturates at very short times unless $\alpha > 1$. We emphasize that $\alpha \geq 1$ corresponds to anomalous dynamic scaling [15], and G grows with time as a power law with a larger anomalous exponent (0.40) in the intermediate time scales than would be predicted by the analytic anomalous scaling behavior (0.25) for Eq. (2) [15]. Note that our definition of G coincides with the mean square step size $C(1,t)$ which is just the $x = 1$ value of the height-height correlation function $C(x,t)$ [14,15]. If the dynamic scaling behavior is anomalous [14,15], then w and G invariably lead to different effective exponents independent of whether α is greater than or less than 1. In this paper, we measure α_{eff} by studying $G = \langle(\nabla h)^2\rangle$ (i.e., the local α_{eff}) which coincides with the α_{eff} measured from $w(t,L)$ studies (i.e., the global α_{eff}) only if the standard dynamic scaling hypothesis applies.

We attempted to obtain rough qualitative values of α_{eff} by looking at G versus t on a log-log plot: in the NU case [Fig. 3(b)], the high-temperature fate of G is saturation consistent with the usual scaling behavior, while for the UD model [Fig. 3(a)] G is still increasing even for $T = 675$ K, clearly showing that the UD model scales anomalously [15] in that such an increase of G requires the globally measured α_{eff} to exceed unity. The saturation of G (implying $\alpha < 1$) in the NU model points to Eq. (1) as being the best description of its interface (there may well be a small λ_{43} term in addition to the most relevant ν_2 term as a higher order effect). Thus we speculate that the NU model belongs to the EW universality class even though a naive study of β_{eff} does not necessarily lead to this conclusion due to the competing finite size effects which are invariably present [4]. Our speculative identification of the NU model at high T with EW growth is thus based on indirect evidence. At this stage, we cannot conclude whether at low T in the NU model we observe anomalous scaling behavior [such as given by Eq. (2)] or simply a smooth crossover with temperature from purely random low temperature growth to the high temperature EW growth (although other simulations [3,4,17] also find β_{eff} near 3/8 when $R_1 \approx R_{dep}$). A crossover in the scaling behavior with

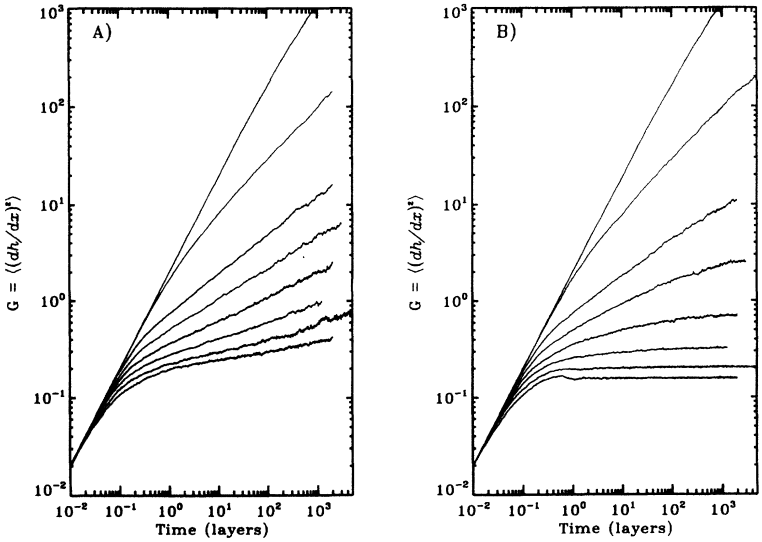

FIG. 3. Plot of $G = \langle(\nabla h)^2\rangle$ as a function of time for various temperatures ($T = 450, 500, 550, 575, 600, 625, 650, 675$ K from top to bottom). $L = 4000$ except for $T = 675$ K ($L = 10\,000$). (a) UD model. (b) NU model.

temperature would be interesting, but is extremely difficult to pin down due to competition from finite size and time effects.

It is more difficult to distinguish the anomalous dynamic scaling of the $\alpha = 1$ and $\alpha = 1.5$ situations due to the slippery nature of the clearly identifying logarithmic behavior and possible problems arising from unknown features in anomalous dynamic scaling. However, Fig. 3(a) shows that the slope of G drops only to 0.1 at $T = 675\,\mathrm{K}$ and $L = 10^4$ for the UD model, so that at least below this temperature, the λ_{42} term does not appear to be dominant. But neither does Fig. 3(a) show a constant slope of $G(t)$ equal to 1/4 to be consistent with the scaling behavior of Eq. (2) which may be expected because of the stable value (≈ 0.35) of β^a_{eff} observed in Fig. 2(a): indeed for $T = 550\,\mathrm{K}$, $G \sim t^{0.41}$. One may retain some measure of reconciliation with the concept of kinetic super roughening proposed by Das Sarma, Ghaisas, and Kim [15] which predicts that $G(t)$ scales anomalously as $G \sim t^{4/10}$ in the discrete Das Sarma–Tamborenea dynamical growth model [3,4] (also called the 1+ model in Ref. [18]). It is now known [14,15] that while the global behavior of this model seems to be controlled by Eq. (2), its anomalous scaling behavior is very different from that of Eq. (2) which predicts $G(t) \sim t^{1/4}$. This quantitative agreement between the Das Sarma–Tamborenea model and our simulations only in the neighborhood of $T = 550$ K may not possess any unique significance. Nevertheless, because of the observation of a stable β^a_{eff} close to that of the fourth order linear continuum equation at that temperature ($T = 550$ K), we are inclined to believe that the UD model (as opposed to the NU model) is displaying anomalous scaling behavior consistent with the Das Sarma–Tamborenea 1+ (or the Wolf-Villain $d2+$) model for $T \geq 500$ K, albeit with a strong temperature dependence of the effective exponent α_{eff}. For temperatures greater than those studied here Fig. 3(a) indicates that $G(t)$ may eventually saturate, in which case any scaling behavior would be of the standard type. Thus the understanding of the continuum equation controlling MBE growth may be intimately tied to our understanding of the continuum equation describing the dynamical Das Sarma–Tamborenea model [3], at least over intermediate time scales. The fact that $G(t)$ may eventually saturate may very well be a finite size effect or may indicate a crossover to EW universality (as in the Wolf-Villain dynamical model [6]). This point clearly needs further investigation [34,35].

To obtain a more conclusive determination of the scaling in the UD and NU models, we have measured the full correlation function $C(x,t) = \langle (h(x+r,t) - h(x,t))^2 \rangle$ and extracted from it the correlation length, ξ, as a function of time. Our operational definition of ξ is the length at which $C(x,t)$ first saturates. In Fig. 4, this data is presented for $T = 500, 600$, and 650 K. In general, the scaling law $\xi \sim t^{1/z}$, where z is the dynamical exponent, holds extremely well over more than two decades in time. The main observation is that the slope of these $\log(\xi)$-$\log(t)$ plots in the UD model changes slowly, from 0.21 to 0.29, over a range of 150 K: on the other hand, the calculated slope in the NU model deviates sharply from its low

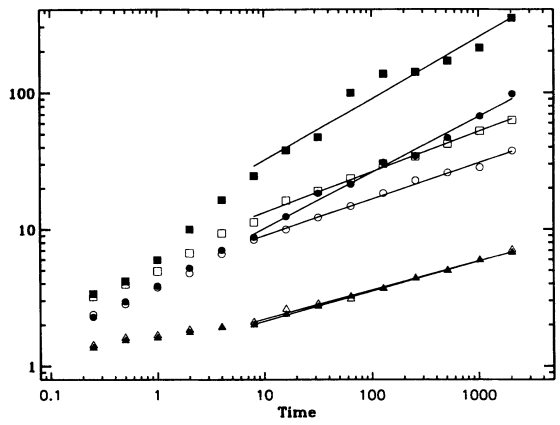

FIG. 4. Plot of the dynamical correlation length versus time for the UD (open symbols) and NU (filled symbols) models at $T = 500(\triangle), 600(\bigcirc)$, and 650 K ($\square$). The best fit lines have the following slopes: $T = 500$ K (UD): 0.21 ± 0.01, $T = 500$ K (NU): 0.22 ± 0.01, $T = 600$ K (UD): 0.26 ± 0.02, $T = 600$ K (NU): 0.41 ± 0.01, $T = 650$ K (UD): 0.29 ± 0.02, $T = 650$ K (NU): 0.43 ± 0.05.

temperature value of 0.22, becoming 0.43 at $T = 650$ K. If we identify this slope with $1/z$, i.e., $\xi \sim t^{1/z}$, which is expected to hold even in the anomalous dynamic scaling case [15], we can obtain the dynamical exponent z. It is interesting to note that for Eq. (2) $z = 4$, close to all slopes in Fig. 4 for the UD model (open symbols) and the low-T behavior of the NU model. Furthermore, Eq. (1) has $z = 2$: the correlation function behavior thus also supports the claim that due to crossover effects the NU model (filled symbols) changes its effective universality for $t \leq 2000$ from that of Eq. (2) to that of Eq. (1) at high temperatures. On the other hand, in the UD model $1/z$ changes from 0.21 (low T) to 0.29 (high T) which is consistent with, but not absolutely conclusive evidence for, the scenario that the low-T behavior of the UD model is given by the linear diffusion equation [Eq. (2)] and the high-T behavior by the nonlinear LDV equation, possessing the $\nabla^2(\nabla h)^2$ term, which has $z = 3$.

Thus, the NU model, after producing a global β_{eff} close to that predicted by the universality of Eq. (2) when R_1/R_{dep} is close to unity, appears to be asymptotically governed by Eq. (1) as activated diffusion gets stronger at higher temperature. When upward hopping is added there is evidence [Fig. 2(a) and Fig. 4] for Eq. (2) (or the nonlinear LDV equation) holding over a much broader range of temperature, with the possibility that the universality class might change for hopping rates higher than those studied here. Also, note that while α_{eff} does continuously decrease with T, we can observe (Fig. 3) slight positive curvature at late times ($t \sim 10^3$) suggesting that G does not saturate just beyond the end of our UD simulation. In contrast, the NU model possesses a $G(t)$ which either saturates or shows a negative curvature. It would be interesting to consider the manner in which the UD model becomes the NU model as the facility of uphopping is reduced in light of the potentially different

scaling laws they follow in the intermediate temperature regime we have investigated.

To quantify the strength of upward hopping in our UD model, we present in Fig. 5(a) the fraction of out-of-plane hops which decrease the height as functions of both time and temperature. The percentage of downward hops remains nearly constant in time although a slight decrease at long times can be seen. Upward hopping, caused by the migration from kink and trapping sites, does not account for more than 10% of all the out-of-plane hops until $T \approx 600\,\mathrm{K}$, but by $T = 675\,\mathrm{K}$ up-hops and down-hops are almost equally likely. A positive, nonzero difference in the absolute number of down-hops and up-hops (per layer), Δ, indicates that hopping on the whole acts to transport atoms towards the substrate: Fig. 5(b) replots the data of Fig. 5(a) to measure this difference. Note that Δ eventually saturates, but requires on the order of 10 layers to do so: this may be related to the early low value of β_{eff}. The value of $\Delta(T,t)$ also appears to saturate to a positive value with increasing temperature as the up-hopping fraction goes to 1/2. This demonstrates a definite bias in favor of hopping towards the substrate even when up- and down-hopping are kinetically equivalent as $\Delta(T,t) > 0$. It is tempting to make a connection between a nonzero Δ and a nonzero ν_2, the driving force in EW growth resulting from forcing atoms to relax to local height minima. But such a direct link fails for the Das Sarma–Tamborenea model (i.e., the 1+ model of Ref. [18]), which has only lateral and downward hops, making $\Delta > 0$ whereas ν_2 is thought to be vanishingly small [34] (even though an extremely small but nonzero ν_2 cannot be ruled out in simulations [14]). One way to conclusively determine whether $\nu_2 \neq 0$ is to measure the surface current in a locally tilted substrate as discussed in Ref. [35]. Such a calculation for our models has not been attempted and is likely to be inconclusive due to very strong finite size (time) effects. The UD model (in addition to the NU model) may very well have $\nu_2 > 0$ and eventually may crossover to the universality class of Eq. (1) in the $L \to \infty, t \to \infty$ limit. This belief that the NU and UD models are likely to both be asymptotically described by the EW universality (i.e., $\nu_2 > 0$) gets additional support from recent work [14,35] which shows that the Wolf-Villain model or the $d2+$ model of Ref. [18] may actually belong to the EW universality class. Since in our stochastic models we allow both singly and doubly coordinated particles to hop, our model is actually closer in spirit to the Wolf-Villain $d2+$ model than to the Das Sarma–Tamborenea 1+ model. At this stage, it is, however, appropriate to consider the asymptotic universality class of the UD model to be an open issue. We have, however, established that the UD model is effectively (as opposed to asymptotically) described by the linear diffusion equation [Eq. (2)] or the nonlinear LDV equation [Eq. (3) with $\nu_2 = \lambda_{43} = 0$], and the NU model is asymptotically described by the EW equation.

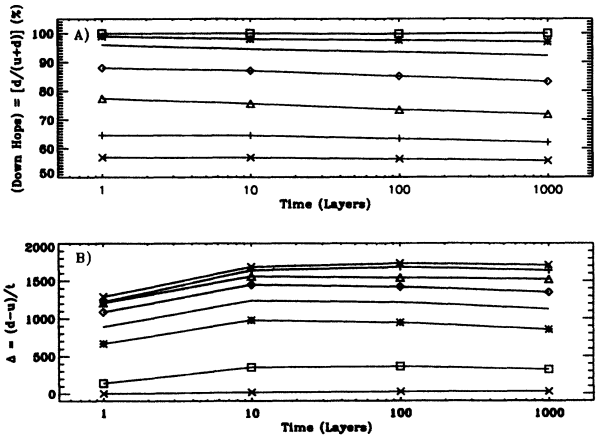

FIG. 5. (a) The percentage of out of plane hops which are downward (lateral hops are not counted) in the UD model as a function of time and temperature [$T = 500(\Box)$, $550(*)$, $575(\cdot)$, $600(\Diamond)$, $625(\triangle)$, $650(+)$, $675\,\mathrm{K}$ (X) from top to bottom]. $L = 10\,000$ for $T = 675\,\mathrm{K}$ and $L = 4000$ for all other T. (b) The same data as Fig. 3(a) [but adding a $T = 450\,\mathrm{K}$ (X) run] replotted as the difference between the absolute number of down- and up-hops (per layer). The temperature increases from bottom to top here.

We note for the sake of completeness that in the NU model Δ (which in this case gives the total number of down-hops per layer) also seems to saturate with t and T, and $\Delta(T = 675\ \mathrm{K},\ t > 10) \approx 1950$ hops/layer. In terms of absolute numbers, for $T = 675$ K and after $t = 10^3$ layers in the UD (NU) model, we observed 8.33×10^6 (1.96×10^6) down-hops, 6.61×10^6 (0) up-hops, and 95.1×10^6 (64.2×10^6) lateral hops. So while the *net* number of downward hops Δ is only a modest 14% higher in the NU model, the presence of up-hops in the UD model greatly augments the total number of lateral and downward hops executed on the surface without greatly upsetting the net flow of matter toward the substrate. Given this, it is initially somewhat surprising that the correlation length is actually smaller in the UD model (Fig. 4). But an atom which hops down has, on its next hop, a chance of returning to its original site only if it can hop up. Thus an up-hopper is akin to a random walker and after n hops will only wander $\sim \sqrt{n}$ sites. If the down-hopper moves same $\sqrt{n}$ sites to reach a lower terrace after n hops, the random walk for this atom begins anew, with the distance it has already traversed no longer reduced, for the atom can never return to the upper terrace. After n' more hops, the up-hopper has wandered $\sqrt{n+n'}$ sites, while the down-hopper has traversed a greater distance, minimally $\sqrt{n}+\sqrt{n'}$. We also note that up-hopping is dominantly a two-bond cutting process, while both down and lateral hopping is dominated by the contribution of highly mobile singly bonded atoms on flat terraces and atop step edges: it is thus energetically more likely that an atom at a step edge will hop as opposed to the doubly bonded atom at a kink. In this way, the Arrhenius rates naturally favor down-hopping over up-hopping.

The last two models we consider completely suppress downwards hopping and should accentuate any features of growth that lead to a diffusion-barrier induced Schwoebel-type instability [28]. When only in-plane hops occur (the LAT model), the width grows with exactly the random growth exponent of $\beta = 1/2$ for all values

of T [18]. In the random deposition case, i.e., $T = 0$ K, the particles' inability to escape their deposition sites produces uncorrelated growth, while here it arises from atoms being confined to randomly chosen "terraces," which from the point of view of long wavelength fluctuations, are equivalent to single (renormalized) sites [18].

Finally, in the ND model, constructed from the LAT model by allowing upward hops (exclusively 2 and 3 bond breaking processes), but no downward hops, we observe $\beta_{eff} > 1/2$. When the upward motion is weak, β_{eff} remains close to the LAT value (1/2), while stronger up-hopping yielded slopes as large as 0.9. The ND model clearly produces an instability (in that $\beta_{eff} > 0.5$, the value for purely random growth) implying a breakdown of dynamic scaling. Notice that β_{eff} peaks near $T = 600$ K ($R_2 = 0.45 R_{dep}$), dropping off slightly as the temperature climbs to 675 K (where the width exceeds the average height). But the ND simulation at high T grows an order of magnitude fewer total layers as compared with the other models, so the values of β_{eff} reported here may not be the asymptotic ones, and this is the cause for the observed decrease. We emphasize also that once $\beta > 1/2$ characterizes the growth dynamics, using critical exponents becomes somewhat of an empty exercise.

Figure 6 summarizes results from all four of our models. Both the models with downward diffusion (UD and NU) show $\beta_{eff} < 1/2$ in all cases, whether accompanied by upward hopping or not. Imposing an impassably high barrier to downward hopping in the absence of upward motion (LAT model), however, causes the fluctuations to grow randomly as $t^{1/2}$, independent of temperature. Setting the barrier to downward hopping at some finite value, therefore, could not conceivably yield an effective exponent β_{eff} outside the bounds set by the NU and LAT models (when up-hopping is forbidden). At $T = 600$ K, we verify this claim in the NU model by imposing an additional downward hopping barrier, E_s, that ranges from

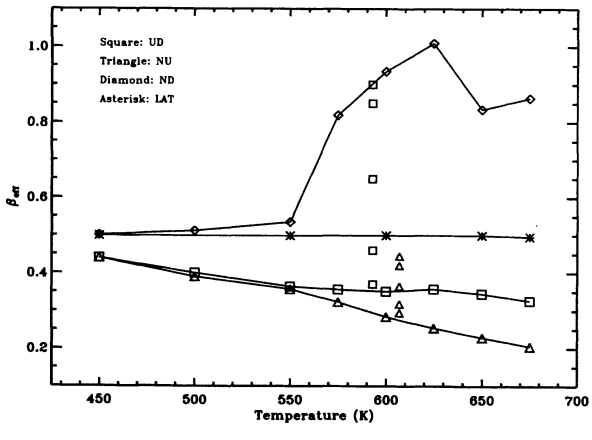

FIG. 6. Late time exponents (β_{eff}) versus temperature in all models: UD (□), NU (△), ND (◇), LAT (*). $L = 4000$ except for $T = 675$ K ($L = 10\,000$). An average over 3–10 runs has been performed. The small boxes show β_{eff} in the UD model when $E_s = 0.003, 0.015, 0.036, 0.12$, and 0.24 eV (from bottom to top) for $T = 600$ K (offset for clarity); the small triangles represent the same data for the NU model.

0.003 eV to 0.24 eV: if the atom cannot overcome the extra barrier then it does not move. The resulting values of β_{eff} are displayed as small triangles in Fig. 6. Note that a 3 meV barrier has a small, measurable effect and $E_s = 0.036$ eV yields a slope exceeding that of the corresponding β_{eff}^{UD}: when up-hopping does not occur, β_{eff} does in fact remains less than 1/2.

When upward mobility is allowed, the possibility of unstable growth emerges as the two limiting cases (the UD and ND models) straddle the $\beta_{eff} = 1/2$ borderline that defines purely random growth, and separates those exponents in principle consistent with an equation such as Eq. (3) from those with no possible dynamic scaling ($\beta_{eff} > 1/2$). Any real growing interface should thus possess an effective exponent less than that of the ND model: for actual surfaces to behave similar to the ND model would require both a sufficiently large energy barrier to downward hopping (measured Schwoebel barriers are typically ~ 100 K), with no barrier to upward diffusion other than the bonding energy. To gauge the effect of a diffusion barrier, we vary E_s from 0.003–0.24 eV (again at $T = 600$ K), upsetting the microscopic balance created by the up-down symmetry when $E_s = 0$. Within the UD model, β_{eff} shows a great sensitivity to impeded downward motion (small boxes in Fig. 6): when the barrier is as small as $E_s = 0.015$ eV (~ 175 K), or the probability of down-hopping is 75%, β_{eff} rises to 0.46, a change induced by a modest 16% drop in Δ. Instability, therefore, can set in, and to see such behavior we had to force the downward hopping to be more difficult than upward hopping for equivalently coordinated atoms. And from Fig. 6, we clearly see the necessity of upward mobility for such an effect, as in no case did the NU model produce $\beta_{eff} > 1/2$. Thus an observation of $\beta_{eff} > 1/2$ in an experiment would seemingly simultaneously suggest the presence of both a Schwoebel-type barrier and upward mobility on the surface. In the absence of any accurate knowledge about the Schwoebel barrier in real semiconductor systems, and given the volatile nature of these models with E_s and the role of upward mobility, we cannot really say much more at the present time.

It seems then that one cannot obtain β_{eff} greater than 1/2 when $E_s = 0$; upward hopping alone is not sufficient to produce an instability. The presence of upward hopping, while drastically increasing the total hopping events, had a much smaller effect on the net diffusional flux toward the substrate. If up- and down-hopping was ignored altogether, the exponent $\beta_{eff}^{LAT} = 0.5$ for all temperatures. The only way we to achieve $\beta_{eff} > 1/2$ within our schemes was to make down hopping more difficult than up-hopping ($E_s \neq 0$). At $T = 600$ K this occurred for $E_s > 0.015$ eV (a factor of ~ 2 or so larger than experimentally observed barriers), and happens at all T for a high enough barrier. We, therefore, speculate that *within* conserved SOS models not possessing a diffusion barrier, MBE growth is generically stable. Of course, this supposed generic MBE growth stability does not rule out unstable growth for a particular material at temperatures where material-dependent parameters cause sufficiently large diffusion barriers which can lead to an instability. In general, we believe Eq. (3) to hold under SOS growth

conditions. For thin films at lower temperatures, the continuously changing β_{eff}, together with a transient whose effective slope continuously changes and a material dependent diffusion barrier, makes an unambiguous determination of the universality class in MBE very difficult, and may in fact be a source of disagreement in the experimentally measured β_{eff} [24,25,27,36] and α_{eff} [26,27].

We emphasize that our simulations are in two dimensions while most real growth measures the $d = 3$ scaling properties. All of the experiments with $\beta_{eff} < 0.5$ estimate effective exponents in the range $\beta \sim 0.2$–0.3, overlapping the range of exponents predicted for various special cases of Eq. (3): from 0.167 (λ_{43} term exists) to 0.25 (if ν_4 term is relevant). Given the numerical similarity of β in these cases, one must be very careful about the nature of any transients and finite size effects that could affect the measured values of the effective exponents. Our results in the simpler $d = 2$ case reflects negatively on the hope that real growth will in fact possess unique, temperature and material independent dynamical scaling behavior consistent with the solid-on-solid approximation, except in the high-T limit, where EW universality, in all likelihood, is operative. And since in $d = 3$ more hopping modes exist due to the higher coordination of atoms, transient behavior should actually become even more of a problem for real growth than it is here in our $(1 + 1)$-dimensional simulations. Indeed, the determination of a single universality class for growth of a particular crystal seems to hold many parameter-dependent complications which at present are hard to quantify with any generality. One should note that for $d = 3$ models, the asymptotically expected EW universality enters as a very weak (logarithmic) divergence of the width in time. Operationally, it will be difficult to differentiate true logarithmic scaling from amongst the influences of finite size effects and decreases in slope due to transients when diffusion is important: monitoring the surface gradient with time is a useful tool to help sort out the asymptotic scaling from these extraneous affects.

To summarize our results we find the following.

(i) Uncorrelated random growth ($\beta = 1/2$) in the LAT model where interlayer hopping (either up or down) is prohibited.

(ii) Unstable growth with $\beta > 1/2$ for the ND model where up-hopping, but no down-hopping, is allowed. Unstable growth is also found in the simultaneous presence of a finite diffusion barrier ($E_s \neq 0$) and up-hopping even if down-hopping (reduced by the diffusion barrier) is allowed.

(iii) Most likely EW asymptotic growth in the NU model where down-hopping, but no up-hopping occurs (this conclusion is indirect, however).

(iv) Anomalous dynamic scaling [14,15] with global $\beta_{eff} \approx 0.35$, $z \approx 4.7$–3.4 in the UD model where detailed balance is explicitly obeyed with both up- and down-hopping allowed in the simulation. Based on indirect evidence relating the UD model to the $d2+$, Wolf-Villain model, we believe that for very high T, a crossover to Eq. (1) [i.e., $\nu_2 \neq 0$ in Eq. (3)] may occur in this model though the issue is by no means settled.

For long intermediate time regime, in temperature ranges of different extent, our UD and NU models seem to have the *global* exponents given by the linear fourth-order surface diffusion equation [Eq. (2)] with some hints (more so in the UD model) of the nonlinear LDV term showing up. We believe that understanding the true dynamical critical behavior of MBE growth remains intimately tied to our first understanding the simple Das Sarma–Tamborenea [3] discrete dynamical growth model, which still eludes a continuum renormalization group explanation [12,14,15,22,34,35].

We conclude by emphasizing that the results of our numerical simulation as presented in this paper bring out one particularly difficult aspect of studying MBE growth dynamics as a scale-invariant kinetic surface roughening phenomenon, namely, that MBE growth dynamics is dominated by several diffusion length scales (or, equivalently, several hopping time scales) which strongly affect the crossover behavior of the growth dynamics. As a function of temperature these crossover scales (i.e., the diffusion lengths or hopping rates) vary exponentially, and therefore, at best, MBE growth dynamics may satisfy the requirement of scale invariance only in narrow material-dependent temperature windows where various finite size (and time) effects are minimized. It is, in fact, possible that one does not satisfy the scale invariance requirement for MBE growth except at the lowest temperature where the deposition process is more likely to be ballistic [30] and the SOS consideration of this paper simply do not apply. We believe that this complicated crossover and finite size effect is the reason behind different MBE growth experiments giving widely different dynamical growth exponents as different groups study different crossover behavior. In summary, we believe that our results show that it is very difficult to draw firm conclusions about dynamical growth exponents based on studies of MBE growth dynamics—because of crossover and transient effects fundamentally inherent in the problem the dynamical evolution of surface morphology in MBE growth may necessarily be somewhat murky and not follow the scale invariant surface roughening paradigm in any straightforward way. Certainly, the scale invariant properties of the surface are not universal for all ratios of deposition to hopping strength. Indeed, we have shown that the detailed energetics of surface dynamics may give rise to smoothly varying effective "exponents." Currently existing experimental results are consistent with this somewhat disappointing scenario. Regardless of the universal scaling issues, however, we have shown that an observation of $\beta_{eff} > 1/2$ generally indicates the presence of upward atomic mobility acting in concert with a diffusional barrier to downward motion. In addition we have argued that most MBE growth dynamics is describable by a continuum equation of the type of Eq. (3) with the magnitude of ν_2 being very small sometimes (effectively zero) provided SOS restrictions apply and diffusion barrier effects are not severe.

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