Surface kinetics and generation of different terms in a conservative growth equation

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(Received 9 January 2003; published 28 July 2003)

A method based on the kinetics of adatoms on a growing surface under epitaxial growth at low temperature in $(1+1)$ dimensions is proposed to obtain a closed form of the local growth equation. It can be generalized to any growth problem where surface morphology is governed by adatom diffusion. The method can be easily extended to higher dimensions. The kinetic processes contributing to various terms in the growth equation are identified from the analysis of in-plane and downward hops. In particular, processes corresponding to the term that breaks $h \rightarrow -h$ symmetry and the curvature dependent term are discussed. Effects of these terms on the stable to unstable transition in $(1+1)$ dimension are analyzed. In $(2+1)$ dimensions, it is shown that an additional asymmetric term is generated due to the in-plane curvature associated with mound-like structures. This term is independent of any diffusion barrier differences between in-plane and out-of-plane migration. It is shown that terms generated in the presence of downward hops are the relevant terms in a growth equation. A growth equation in closed form is obtained for various growth models introduced to capture most of the processes in experimental molecular beam epitaxial growth. The effect of dissociation is also considered and is seen to have a stabilizing effect on growth. It is shown that for uphill current the growth equation approach fails to describe the growth since a given single equation does not apply over the entire substrate.

DOI: 10.1103/PhysRevE.68.011605 PACS number(s): 81.15.Aa, 68.55.Ac

I. INTRODUCTION

The growth of a solid phase from vapor has been studied over many years because of its applications in various fields. In particular, vapor phase epitaxial growth has influenced many important technological advances. Such growth is known to be far from equilibrium [1,2]. It therefore offers an opportunity to study the nonequilibrium phenomenon in an experimentally controllable environment. Under these conditions, on the growing interface, processes such as island formation, dissociation, and nucleation do not equilibrate, since they are limited by insufficient mass transport. The resultant interface described by height function $h(\mathbf{r},t)$ develops characteristic correlations on the surface. The study of space time evolution of these correlations constitutes a major aspect of understanding the nonequilibrium behavior of the growth. The continuum equation approach is used to understand this phenomenon [1,2]. This approach helps to obtain the characteristic exponents α, β, and z. α characterizes the spatial variation of roughness as r^{α}, the time evolution is given by t^{β}, and the growth of correlation length by $\xi \sim t^{1/z}$. Under most of the conditions in experimental growth, evaporation and the vacancy formation are negligible [3] implying volume conservation. A conservative growth equation satisfying Langevin equation $\partial_t h + \boldsymbol{\nabla} \cdot \mathbf{J} = F$, where $\mathbf{J}$ is the current due to the adatom relaxation on the growing surface and F is the average flux with white noise, should describe the time evolution of the height function. In order to understand the growth behavior through continuum equation approach, it is necessary to establish the correspondence between surface kinetics and the terms appearing in the equation. This correspondence should corroborate with experimental observations. Experiments in this field show a great variety of results [1,2]. However, initial surface roughness, impurities in the flux, and similar phenomena [4] are inputs to the growth that are uncontrolled in nature. Therefore, their influence on the growth cannot be determined reliably. Simulational studies, that use physical processes as inputs, can be of help in establishing the form of growth equation in a reliable way. In the present paper, we have used computer simulations to verify the implications of different forms of growth equation. The application of these results to real life experiments are discussed in Sec. VI where the experimental conditions such as flatness of the substrate, uniformity of the flux over the substrate, etc., are assumed to be same as corresponding conditions in the simulation.

Based on the experimental observations and computer simulations [5,6], it is seen that when relaxation is governed by surface diffusion of adatoms, at least three terms are expected to contribute to the current: a slope dependent term, an asymmetric term breaking $h \rightarrow -h$ symmetry, and a term proportional to the gradient of curvature [6,7]. The last term will be henceforth referred as ''Mullin's term'' [8]. This term gives rise to a fourth-order term in the growth equation. One of the early efforts [9] used the ''master equation approach'' also referred as the ''microscopic theory,'' for the model involving desorption and column diffusion as the relaxation mechanisms for adatoms. This approach yields slope dependent term *solely* due to the desorption and also the asymmetric term along with Mullin's term due to the surface diffusion. The terms are obtained under small slope approximation. The behavior at large slopes is not clear. Further, it is not possible to establish an unambiguous correspondence between the kinetic processes, and the terms in the growth equation by master equation approach. Kinetic approach involving Arrhenius model or Burton, Cabrera, and Frank (BCF) [10] approach, including nucleation and step edge barriers, does not yield a closed form for the growth equation [2]. It does, however, relate the slope dependent term to diffusion of adatoms on the terrace of a step. Further, to obtain the asymmetric term a quadratic slope dependence

for density of adatoms has to be assumed additionally. Both the terms are obtained under small slope approximation. Using this form, it is not possible to arrive at any closed form of equation describing growth at higher slopes. The Mullin's term is argued to be generated through step detachment [5] or due to the nucleation, based on dimensional analysis [6,7]. This is concurrent with the microscopic theory which attributes the asymmetric and Mullin's term to surface diffusion [9]. Based on the microscopic theory, surface diffusion *always* creates asymmetric and Mullin's terms. Step detachment and nucleation are a result of the surface diffusion process, and they produce these terms. Apparently, there are several processes that seem to be associated with one or more of the growth terms. These processes, however, satisfy the sufficiency criteria for the existence of these terms. It is not clear , whether some of these processes or new ones are necessary for the existence of these terms in the growth equation or not. In this sense, the correspondence between growth processes and terms in the growth equation has not been completely established. As has been noted in Ref. [7], a systematic derivation of surface current is lacking. The work described in the following sections addresses this problem and establishes the correspondence at least within the framework of simple kinetic arguments.

We consider in-plane and downward hops as the basic relaxation mechanism that produce the kinetic processes, giving rise to terms mentioned above. So far, role of such hops has not been explicitly considered in most of the work on growth. Distinctive effects of such hops have been considered in connection with specular spot oscillations in reflected high energy electron diffraction experiments [11], and also while considering their effect on time exponent β [12] in stochastic growth. In the method described in the following section, various terms are obtained by considering the current, as affected by geometrical configuration relevant to the relaxation rules. Here, we calculate the particle current in a heuristic way accounting for the processes generated by in-plane and downward hops by adatoms. This approach is less rigorous compared to the previous ones [2,9]. However, it allows association of the terms in the growth equation with kinetic processes directly. *This isolation of kinetic processes and their association with the terms in a growth equation is the main contribution of the proposed method.* In $(2+1)$ dimensions, an additional asymmetric term due to the in-plane curvature is obtained. This term has relatively weak dependence on the Schwoebel (SE) barrier [13] encountered by a hopping adatom while crossing a step edge. Further, based on computer simulations in $(1+1)$ dimensions, curvature dependent term is argued to be related to the *downward* hopping.

We apply this method to some of the well studied models namely, the Das Sarma–Tamborenea (DT) model [14], the Wolf-Villain (WV) model [15] designed to understand the low temperature molecular beam epitaxy (MBE) growth and also for a model used by Lai–Das Sarma, the LD model [16] to demonstrate the manifestation of Lai–Das Sarma–Villain (LDV) equation. For the DT model without noise reduction, closed form of the growth equation is not known, while in the LD model, the growth equation is empirically related.

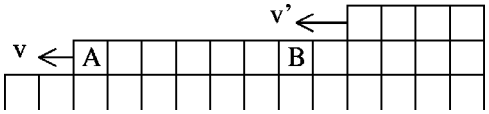

FIG. 1. A typical step structure formed during growth along positive slope. v and v' are velocities of the steps.

Present method allows a closed form of the growth equation for the DT model and also shows how the rules in the LD model produce a term in the growth equation that has similar behavior as the Lai–Das Sarma–Villain equation. Further, once the process to term correspondence is established, it allows us to analyze the growth under uphill current, i.e., unstable growth. It is shown that continuum equation approach fails [17] in such a situation. In Sec. VI, we discuss the relevant results that support the argument of the breakdown of continuum approach.

II. EQUATION FOR GROWTH WITH SURFACE DIFFUSION

Consider growth on a one-dimensional flat substrate with lattice constant *a*. Also assume steps developed as a result of initial growth. We will consider the situation depicted in Fig. 1 for obtaining various contributions to the current where steps are such that positive slope is obtained. Here, the underlying assumption is that the rough or unstable surface will mainly consist of stepped regions. Adatoms are randomly deposited on the substrate. Let D_s be the diffusion constant on the terrace and l_c be the average distance that an adatom travels on a terrace before encountering another adatom. Detachment from steps or nuclei on the terrace is assumed to be negligible. Since the $(1+1)$-dimensional surface essentially consists of steps, we consider kinetics of adatoms on and across the steps. The kinetics is defined through the given set of rules for relaxation of adatoms. Different terms in the growth equation are derived by obtaining the expressions for particle current due to the hopping adatoms and step movement. An adatom contributes to the current through the hopping process, either in the direction of slope (downhill) or opposite to it (uphill). A hop contributes to the current provided the configuration changes between the initial position and the final one. The relevant configuration is decided by the rules of relaxation. In the diffusional relaxation, a hop contributes to the current *only when the number of nearest neighbors* (n_n) *changes, during hop*. We further differentiate between the current due to the downward and the in-plane hops. Adatoms that are hopping down the descending steps contribute to the downward current j_d, while those hopping on the terrace can get attached to an ascending step and contribute to the in-plane current j_i. As inferred from Fig. 1, the adatoms reaching site *A* from the terrace on its right and hopping down the step to the left contribute to j_d. Those reaching site *B* from the terrace on the left of *B* and hopping to the right toward the ascending step contribute to j_i. The net current is j_d+j_i. These are obtained in a mean field approach as follows:

$$j_{d(i)} = [\text{local density of site } A(B)] \times [\text{flux of adatoms approaching } A(B)] \times [\text{probability for hopping across } A(B)]. \quad (1)$$

From the location of the sites A and B in Fig. 1, it is clear that the density of sites A and B is same as the density of steps (effective step height per unit length along the substrate). For small slope, $|m|$ *is* the density of uniform steps [18]. On an ideal surface, as the slope increases step width reduces while step height remains constant. On such a surface, the step width is equal to the single lattice constant for $|m|=1$. The width cannot decrease further. Hence, for slopes higher than unity, the width remains constant and the height increases. Since the number of steps per unit length is same as the number of step widths per unit length, the step density saturates for $|m| \geqslant 1$. However, on a growing surface due to the step width fluctuations, the saturation does not occur at $|m|=1$. To account for these fluctuations and appropriately interpolate for large and small slopes, we have chosen the functional dependence of the step density as $|m|/(1+|m|)$, where m is the local slope. In the limit $|m| \to 0$, this density approaches zero. However, Elkinani and Villain have shown [19] that a "plane" substrate will actually consist of terraces of an average length l_{av}. This will introduce an additional small factor in the numerator of the expression for the density. We will, however, consider the diffusion and deposition rates such that the length $(D_s/F)^{1/4} < l_{av}$ [2]. Under this condition after few monolayers (MLs) of growth, terraces are shorter than l_{av}. The above choice of diffusion and deposition allows us to use the expression for the density of steps as $|m|/(1+|m|)$.

In the absence of nucleation, average lateral flux approaching site B or A is $\pm \hat{\boldsymbol{n}} F/2|m|a^{-1}$ [2]. $a|m|^{-1}$ is the average local terrace width and $\hat{\boldsymbol{n}}$ is unit vector in the x direction. As $|m| \to 0$, flux $\to \infty$. In real systems, this flux is restricted due to the nucleation. The nucleation process will restrict the diffusion of adatoms to an average length l_c on a large terrace. As a result, the effective terrace width does not increase beyond l_c when $|m| \to 0$. Then, the flux is almost constant. The effect of nucleation is incorporated by introducing l_c in the expression for the flux as $\hat{\boldsymbol{n}} F/2(l_c^{-1} + |m|a^{-1})$, so that for small slopes the expression is reduced to a constant value. Let P_A and P_B represent the probabilities of hopping across sites A and B, respectively. The Schwoebel length [20,13] $l_s \propto (P_B - P_A)$. In Ref. [19] it is shown that, if there is a large asymmetry between the sticking coefficients, distribution of diffusing adatoms on the terrace depends upon terrace width. This suggests that P_A and P_B may depend on m for larger asymmetry and shorter terraces. However, when $P_A \to 0$ and $P_B \to 1$, i.e., the case of large SE barrier, the nucleation becomes significant since it is proportional to the adatom density [21]. As a result, the asymmetry of the adatom density on the terrace is reduced, rendering P_A and P_B almost independent of the terrace width. When $P_A = P_B$, there is no asymmetry in the terrace distribution. Under this condition also, P_A and P_B are independent of the width. This suggests that the said dependence is weak. We will therefore neglect this dependence since most of our discussion will be around $P_A \approx P_B$. Further, such an asymmetry is significant when $P_B > P_A$, since it will produce uphill current and large local slopes with shorter terraces. It will be shown that under these conditions, the continuum equation approach fails [17]. Therefore, these probabilities could be considered independent of m where the growth equation approach is valid. Substituting expressions for flux, site density in Eq. (1), we obtain the slope dependent current

$$\mathbf{j}_s = \frac{\hat{\boldsymbol{n}}|m|F(P_B - P_A)}{2(1+|m|)(l_c^{-1}+|m|a^{-1})}. \quad (2)$$

Next we obtain the asymmetric term by noting that the flux approaching sites A and B can be modified due to the relative motion of the steps. Consider the situation in Fig. 1, where v is the velocity of the step bearing the terrace while v' is the velocity of the neighboring step on the higher side. For $v' > v$ the terrace width is reduced, thereby depleting the flux approaching sites A and B. The reduction in flux is δv, where $\delta v = (v' - v)$. Adatoms hopping across upper step as well as those getting attached in plane both contribute to the velocity of the step. Thus, the velocity $v \propto j_s$ with the difference that the coefficient $(P_B - P_A)$ in expression (2) is replaced by $(P_A + P_B)$. Hence, the reduced flux

$$\delta v = \frac{F(P_A+P_B)}{l_c^{-1}+|m|a^{-1}} \partial_x \frac{|m|}{2(1+|m|)(l_c^{-1}+|m|a^{-1})}.$$

Corresponding current *will not depend on* $(P_B - P_A)$, since it represents the amount of the flux removed from the terrace. The current is therefore obtained by multiplying the reduced amount of flux by density of steps. The relative movement of steps causes increase in the local slope for negative curvature on positive slope. This shows that the direction of the current due to the lost flux is same as uphill current which also tends to increase the local slope [22]. P_A and P_B are relative probabilities so that $P_A + P_B = 1$. Applying these arguments for positive curvature on positive slope, one obtains $v' < v$, thereby increasing the terrace size and hence, the lateral flux. Using the same arguments as above it is seen that the expression for this flux is same as that for the case of reduced flux δv as before. Corresponding current is obtained by multiplying the flux by $(P_B - P_A)$ and step density. This current is in the opposite direction compared to the current due to the reduced flux. Accounting for this effect, the expression for the current including the asymmetric term becomes

$$\mathbf{j}(x) = \frac{\hat{\boldsymbol{n}}|m|F(P_B-P_A)}{2(1+|m|)(l_c^{-1}+|m|a^{-1})} + \frac{\hat{\boldsymbol{n}}F[1-(P_B-P_A)]}{2} \partial_x \left(\frac{|m|}{(1+|m|)(l_c^{-1}+|m|a^{-1})} \right)^2. \quad (3)$$

In the limit of small m, the current reduces to

$$\mathbf{j}(x)=\hat{\mathbf{n}}F(P_B-P_A)|m|l_c/2 + \hat{\mathbf{n}}F(l_c^2/2)[1-(P_B-P_A)]\partial_x(m^2). \quad (4)$$

In particular, the second term is proportional to $\nabla(\nabla h)^2$. This term is derived using the BCF theory assuming that at small slopes the particle density on the terraces depends on the even powers of local gradient [2,6]. Further, in Ref. [16] it was conjectured that such a term can arise due to the differences in the velocities of the steps near the top and the bottom of a profile. In the limit of large slope, $|m|a^{-1} \gg l_c^{-1}$ the second term is proportional to $(1/m^3)\partial_x m$. This expression exactly matches with the one derived for large slopes in reference [6]. Thus, the geometrical dependence of the symmetry breaking term in Eq. (3) exactly matches with the previously derived two terms in the small and large slope limits. This shows that the asymmetric term in Eq. (3) appropriately interpolates through the limits of small and large slopes implying the correct analytical form of the term.

Under the infinite SE barrier, i.e., $P_B=1$ and $P_A=0$, the asymmetric term becomes zero. From computer simulations, it is observed that the growth morphology in (1+1) dimensions is symmetric with respect to the $h\rightarrow -h$ transformation, while in (2+1) dimensions it is asymmetric [23,24]. The structures formed during growth do not grow laterally. It has been suggested [25] that asymmetric term does not vanish for infinite barrier. It, however, decreases faster than the slope dependent term which dominates to render a symmetric profile in (1+1) dimensions. However, our analysis shows that in (1+1) dimensions the asymmetric term is absent. We show below that in (2+1) dimensions the in-plane curvature gradient generates an additional asymmetric term. This additional term is not sensitive to P_A and P_B.

In (2+1) dimensions when mound-like structures are formed, steps on the mounds have *in-plane curvature*. The in-plane curvature is given as $\kappa(x,y)=[h_{xx}h_y^2-2h_{xy}h_xh_y+h_{yy}h_x^2]/(h_x^2+h_y^2)^{3/2}$, where, h_x, h_y are derivatives of the height function $h(x,y)$ with respect to x and y, respectively. Consider a region where (i) steps form concentric arcs, (ii) $P_B \geqslant P_A$ and (iii) surface diffusion is isotropic . Under such conditions *the inward flux is proportional to* R^{-1}, where $R=|\kappa|^{-1}$ is the radius of curvature at the point under consideration. In such a region, the relevant velocity of propagation of steps is along the radius of curvature. For a mound-like structure, the radius decreases as the height increases along the mound profile resulting into a *positive* curvature gradient and hence, a velocity gradient. As has been explained earlier in connection with the asymmetric term, this will lead to the reduction in flux. Since the flux in this case is directly proportional to $|\kappa|$, the reduction is given by

$$\frac{c'Fa\left(\frac{\nabla h}{|\nabla h|}\cdot\nabla\right)|\kappa(x,y)|}{2(l_c^{-1}+a^{-1}|\nabla h|)},$$

where c' is a constant of proportionality, $[(\nabla h/|\nabla h|)\cdot\nabla]$ is the gradient in the direction $\nabla h/|\nabla h|$ $(l_c^{-1}+a^{-1}|m|)^{-1}$ is the step width across which the gradient is considered. The current is obtained by multiplying this flux by the step density. Thus, we find that the current due to the difference in in-plane curvature across consecutive planes is

$$j_{cur}=\frac{\nabla hFac'\left(\frac{\nabla h}{|\nabla h|}\cdot\nabla\right)|\kappa(x,y)|}{2(1+|\nabla h|)(l_c^{-1}+a^{-1}|\nabla h|)}. \quad (5)$$

This term will be present *in addition* to the one, due to the curvature in the height profile. For small slope conditions j_{cur} gives

$$\nabla\cdot\left[\nabla hFac'\left(\frac{\nabla h}{|\nabla h|}\cdot\nabla\right)|\kappa|\right]$$

term in the growth equation. Under scaling transformations, this term gives $z-4$, which is same as $\nabla^4 h$ term, but unlike the $\nabla^4 h$ term, it breaks the $h\rightarrow -h$ symmetry. This shows that for the growth near tilt independent (TI) current in (2+1) dimensions mounds grow in time as $t^{1/4}$. The resultant morphology is such that $h\rightarrow -h$ symmetry is broken. Thus, our analysis shows that, for an infinite barrier, in (1+1) dimensions asymmetric term is zero, while in (2+1) dimensions in-plane curvature gradient generates asymmetric term. In fact, in almost all (2+1)-dimensional growths, asymmetry due to this term is unavoidable if mound formation occurs.

We further argue that the Mullin's term must be present in any adatom relaxation process that involves downward hops across the descending step edges. This argument is based on the observation that, in a (1+1)-dimensional simulation, if adatoms are restricted completely to the in-plane hops (infinite SE barrier) then correlations do not grow beyond the diffusion length. This results in the ''wedding cake'' type morphology with fixed size of the ''cakes'' that do not grow laterally in time [23,24] as mentioned earlier. On the other hand, when such hops are allowed, correlation length for stable growth and mound size for unstable growth increases in time [12]. This observation allows one to conclude that height-height (h-h) correlations *increase only in the presence of downward hops*. The microscopic theory [9] predicts fourth-order and asymmetric terms to be present whenever there is a difference in the potential energies (of the adatom), corresponding to its initial and final sites, during a hop. This implies a change in the nearest neighbor configurations between the two sites. Thus, downward hops produce these terms and so does the in-plane hops. In order to differentiate between the role of in-plane and downward hops in generating these terms, consider a rough surface obtained after deposition of several monolayers. We consider an in-plane hop and a downward hop. Let W_i and W_f be the initial and final widths with $W=(1/N)\Sigma_j(h_j-\overline{h})^2$. Also let $G_i(|l-k|)$ and $G_f(|l-k|)$ be initial and final height-height correlations. Consider a hop from site i to $i+1$. The in-plane hop gives $W_i=W_f$, while downward hop gives $W_i-W_f=2a^2$ for an initial single step height difference between the sites i and $i+1$. Thus, the width is reduced due to the downward hop. In order to see the effect on h-h correlations, we consider contributions from the relevant participating sites. Thus, con-

tribution to $G_i(|i-j|)$ will be from sites at h_i, h_{i+1}, h_j, h_{j+1}, and corresponding reflection sites in i and $i+1$. The difference $G_i(|i-j|)-G_f(|i-j|)$ due to one set of sites is $2a^2-2a(h_j-h_{j+1})$. The ensemble average for this process will yield $2a^2$ as the difference. Same contribution will appear from reflection sites. Thus, $G(|i-j|)$ is reduced by $4a^2$ by a downward hop. On the other hand, in-plane hop does not change $G(|i-j|)$, as can be verified by applying the same procedure. This shows that, *in order that correlations grow in time, downward hops are necessary*. The in-plane hops reduce the deposition noise in a plane. Consider a large flat surface with very small coverage. Every event of an adatom getting captured by a nucleus or another adatom causes decrease in $G(1)$. The values $G(1),G(2),\ldots,G(m)$ for m atoms forming an island are less than their corresponding values for m isolated atoms. This indicates reduction of noise in a plane. In fact, this process develops correlations over the diffusion length l_d. In Ref. [9], it is shown that fourth-order and asymmetric terms are generated whenever nearest neighbor configuration is changed in a hop. This is consistent with the reduction in $G(m)$, $m \leqslant l_d$ with hops leading to increase in near neighbors while attaching to the islands. Thus, in-plane hops do generate fourth-order and asymmetric terms, however, these exclusively operate within l_d reducing deposition noise in a plane. The processes such as nucleation and step attachment or detachment [20,7] are suggested to generate fourth-order term. The above discussion leads to the conclusion that term generated due to these processes will operate only within the plane and not across different planes. This shows that *in a growth equation, terms generated by the kinetic processes involving downward hops are the relevant terms*. This also suggest that upward hops will *decrease* the correlations. We do not consider in the present work effects associated with upward hops, as we restrict the analysis to the low temperature growth. From expression (2) and Fig. 1, downward hops crossing site A will generate downhill current. Hence, if the downward hops are allowed and the current is tilt independent, then it may be expressed as a linear combination of higher derivatives, $a_1\nabla^3 h + a_2\nabla^5 h + \cdots$ including the nonlinear terms of the form $\nabla(\nabla^3 h)^2$. Here, the signs of the coefficients $a_1, a_2, \ldots$ are such that the corresponding growth equation describes a stable growth. We will retain only $\nabla^3 h$ in the current corresponding to our minimal growth equation. Thus, the form of the current corresponding to such an equation in $(1+1)$ dimensions is

$$\mathbf{j}(x) = \frac{\hat{\boldsymbol{n}}|m|F(P_B-P_A)}{2(1+|m|)(l_c^{-1}+|m|a^{-1})} + \frac{\hat{\boldsymbol{n}}|m|F(1-P_B+P_A)}{2}\partial_x\left(\frac{|m|}{(1+|m|)(l_c^{-1}+|m|a^{-1})}\right)^2 + \nu\frac{\partial^3 h}{\partial x^3}. \tag{6}$$

The first term has been studied widely in the context of stable growth [26,27] and unstable growth mode [28]. We aim to study TI current models here. This will allow us to study the exclusive effect of asymmetric term. With this view we have performed simulations of a $(1+1)$-dimensional solid-on-solid model with *no diffusion bias* (i.e., $P_A=P_B$). This will produce growth with TI current. A fourth-order equation was earlier proposed by Villain [20] for similar situation. Under this condition, the first term in Eq. (3) vanishes. The resultant growth equation in the moving frame with growth front is of the form

$$\partial_t h = -\nu\frac{\partial^4 h}{\partial x^4} + \nu_a\partial_x^2\left(\frac{m}{(1+|m|)((l_c^{-1}+|m|a^{-1})}\right)^2 + \eta, \tag{7}$$

where ν_a is the appropriate constant for the asymmetry term and η is white noise associated with deposition flux with $\langle\eta(x',t')\eta(x,t)\rangle = D\delta(x'-x)\delta(t'-t)$. In the limit of small slopes, renormalization group analysis shows that the roughness exponent $\alpha=1$, the roughness evolves with the exponent $\beta=1/3$ [16] and growth exponent for correlation length $z=3$. For large slopes, when terrace width is very small (of the order of a), it is shown in Sec. V that the asymmetric term in Eq. (7) gets modified due to the discretization effect. The resultant term leads to the scaling exponents $\alpha=1.5$, $\beta=3/8$, and $z=4$. This term describes the DT model [14] in the absence of noise reduction. We discuss the growth equation for the DT model in Sec. III A. Here, we note that in the limit of large slopes Eq. (7) will reduce to the equation describing the DT model, hence exponent β should cross over from a value of 1/3 to 3/8. In the following section, we describe a solid-on-solid growth model that mimics the relaxation by surface diffusion. The relaxation rules are consistent with the processes giving rise to different terms in Eq. (6). These results will help to establish the relationship between process→term in a growth equation. In Sec. V, we apply this method to predict growth equations for other models.

Corresponding growth equation in $(2+1)$ dimensions is obtained from similar kinetic considerations. These considerations show that for isotropic diffusion, same form as Eq. (6) is obtained by defining $\hat{\boldsymbol{n}}=\nabla h/|\nabla h|$, replacing length-derivative product in asymmetric term by $\nabla h\cdot\nabla/(l_c^{-1}+|\nabla h|)|\nabla h|$, and adding the asymmetry term due to the in-plane curvature gradient. For small slopes one obtains $\nabla(\nabla h)^2$ term [16] along with $\nabla\cdot[\nabla h(\nabla h\cdot\nabla)|\kappa|]$, which seems to describe many experimentally observed growth roughness measurements from vapor [29]. In particular, in large number of experiments the roughness exponent α is seen to be in the range of 0.65–1.0 which is close to the predictions by these two terms.

III. GROWTH MODEL

Growth with surface diffusion and dissociation

This model can be described as follows. Atoms are rained on a one-dimensional substrate of length L randomly with constant flux. On deposition a given adatom is allowed to hop n times, as in a random walk. The hops can be biased through a parameter p. Thus, $p=1.0$ is the growth with infi-

nite positive SE barrier, while $p=0.0$ is with infinite negative barrier. We assume $p=1/2$, i.e., no bias condition for most of the cases. If the hopping adatom has $n_n \geqslant 2$, before n hops are exhausted, the adatom is incorporated. If n hops are exhausted without encountering any nearest neighbor, it stays permanently at the last position occupied after n hops. For a case where a hopping adatom encounters $n_n=1$, we define another parameter q. The parameter q decides fraction of such events, where adatom will dissociate from its neighbor. For $q=0$, detachment is completely suppressed. Under this condition detailed balance is not obeyed. As usual, q is compared with the random number to decide whether detachment can take place or not. We have extended the same model in $(2+1)$ dimensions. Besides the parameters p and q that control the hops across the step edge and away from the edge, respectively, an additional edge diffusion has been included [30]. It is considered to be intraplanar process. We also employ the noise reduction method [31] whereever needed. In this method, after deposition an adatom is allowed to make hops as per the rules until it finds the location for the incorporation. However, instead of actually incorporating the atom at that position, a counter at that position is increased by unity. A given position is filled only when the counter exceeds a certain predecided number. The method has been successful in bringing out the correct nature of the growth at earlier times in simulation [32]. We find that when the number of allowed hops are large enough, noise reduction occurs in the diffusion process during initial growth.

The present model includes the physical processes dependent on the surface diffusion. It, however, differs from kinetic Monte Carlo (KMC) method, usually employed in such simulations. First, the detailed balance is accounted in KMC since dissociation from the steps or nuclei is allowed as per the activation barrier for that event. The dissociation from steps is in opposite direction to that of attachment from site B in Fig. 1. Fraction of the dissociated atoms will diffuse across the terrace and hop downward. This will constitute additional downhill current. This current however, is, *independent of terrace width* and depends only on the density of edges (the details are discussed in Sec. IV B). As a result, the slope dependent uphill current decreases with slope while dissociation induced downhill current does not. This leads to TI current. We will illustrate this effect in the following section. KMC method also allows upward hops and edge diffusion. Thus, based on the considerations of contributing currents, KMC method would tend to TI current growth rather than a true uphill current. The present model however, is, computationally convenient in that, it allows variation of parameters in such a way that isolation of processes and their effect on growth equation can be studied. By adjusting parameters in our model, downhill, zero, or uphill current can be maintained during growth simulation. For comparing the predictions of growth equation with simulations, we have measured width W, height-height correlations $G(\mathbf{r},t)$ and skewness σ, where $W=(1/N)\Sigma_i(h_i-\overline{h})^2 \sim t^{2\beta}$ and $G(\mathbf{r},t)=(1/N)\Sigma_{\mathbf{r}'}[h(\mathbf{r}+\mathbf{r}',t)-h(\mathbf{r}',t)]^2$. The skewness $\sigma=w_3/W^{3/2}$, where $w_3=(1/N)\Sigma_i(h_i-\overline{h})^3$ [33].

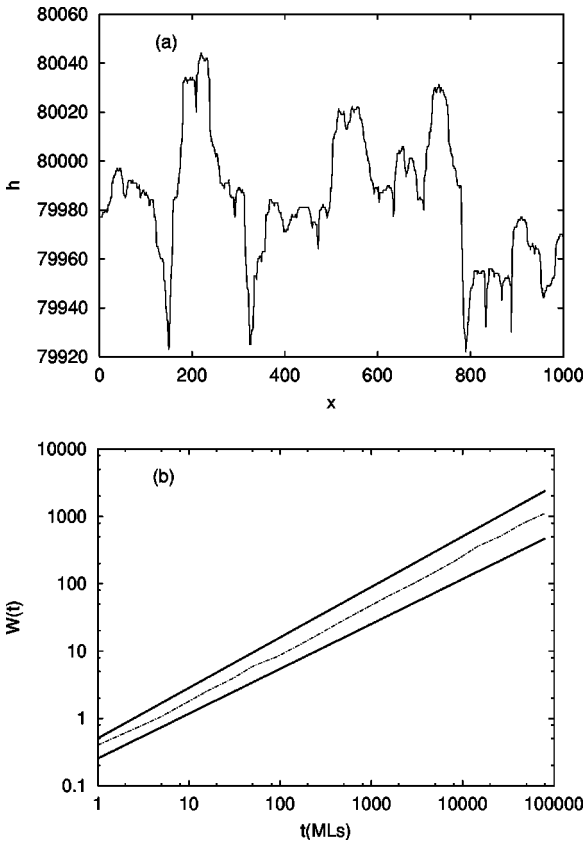

FIG. 2. (a) Morphology of the surface after 80 000 number of layers. Height h and distance x are measured in lattice units. (b) Plot of width as a function of time. Thicker lines with slope 3/4 and 2/3 are drawn for reference. Time is measured in units of number of monolayers (MLs) for a constant flux. The substrate size is 10 000 and SE barrier parameter p is 0.5 (i.e., no SE barrier).

IV. RESULTS

A. TI current without dissociation

From the derivation of expression (6), it is clear that TI current is obtained when $p=0.5$ and $q=0$, allowing $P_A=P_B$. Thus, mainly two terms are expected to contribute in the growth equation, the $\nabla^4 h$ and the asymmetric term. Presence of $\nabla^4 h$ term is verified from the flatness of the saturated width for small L. We have chosen $n=10$ giving $l_c \approx 3$. The saturated width is observed to be flat almost up to $5l_c$, showing that $\nabla^4 h$ dominates at small lengths [6]. Figure 2(a) shows the morphology of the interface after 80 000 MLs are grown. As predicted by Eq. (7), the asymmetry is evident in the figure with $\sigma=-0.31\pm0.05$. Figure 2(b) shows plot of W vs time. We obtain initially β around 0.33 that attains a value of 0.35 ± 0.015. Initial value of 0.33 matches well with the predicted one by the Eq. (7), in the limit of small slopes (compare data in the region from 10 ML to 200 ML in the figure with the line having slope of 2/3). Correspondingly, h-h correlations lead to the roughness exponent α that increases from 0.5 to 0.75 ± 0.01 over a growth of 10^3 to 4×10^6 MLs. Clearly, α tends to unity asymptotically on large substrates. The value of α from saturated width and for small n is 1.35 ± 0.1. These results indicate

that most of the morphological features of the growth with diffusion without detachment are captured by the growth equation (7). As mentioned in Sec. II, a slow crossover from $\beta=1/3$ to $\beta=3/8$ is observed. The exponent α from W_{sat} is also close to the predicted value of 1.5 [14]. Thus, the model in Sec. III represents the growth equation given by Eq. (7) confirming the association of kinetic processes with the terms in the growth equation. It also shows that diffusion of the adatoms roughens the growing surface. Diffusion bias causes additional effects such as stability or instability of growth. In particular, if the bias is varied from extreme negative SE barrier to extreme positive SE barrier, a stable→unstable transition is observed. In this transition, however, $h\rightarrow -h$ symmetry is broken asymptotically. Note that in the stable region, for negative SE barrier, $\nu_2\nabla^2 h$ term dominates with positive value of ν_2 [26], so that asymptotically asymmetric term becomes irrelevant, rendering $\sigma=0$. At exactly zero SE barrier, finite negative value of σ is obtained. In the unstable region with positive SE barrier $\sigma\leqslant 0$. σ can be regarded as the symmetry parameter that changes abruptly at the transition point. Thus, the stable→unstable growth transition for this model with $q=0$ is like second order phase transition. This transition is, however, a result of not complying with detailed balance.

As mentioned earlier, in (2+1) dimensions, TI current growth could not be obtained by putting $P_A=P_B$. We could attain a situation close to the TI current growth by setting the parameter p to a value 0.54, and without edge diffusion. Results in Fig. 3(a) show the morphology, where mound-like structures are evident, while Fig. 3(b) shows plot of position of first maximum in $G(\mathbf{x},t)$ vs time. From Fig. 3(b), we obtain the exponent $1/z=0.23\pm 0.02$. We have measured β to be 0.26 ± 0.03 and $\sigma=-1.12\pm 0.1$ for this model. These results clearly indicate an asymmetric term leading to the value of the exponent $z=4$. As has been discussed previously, it is the term generated from the the current j_{cur} in Eq. (5), governing the growth dynamics.

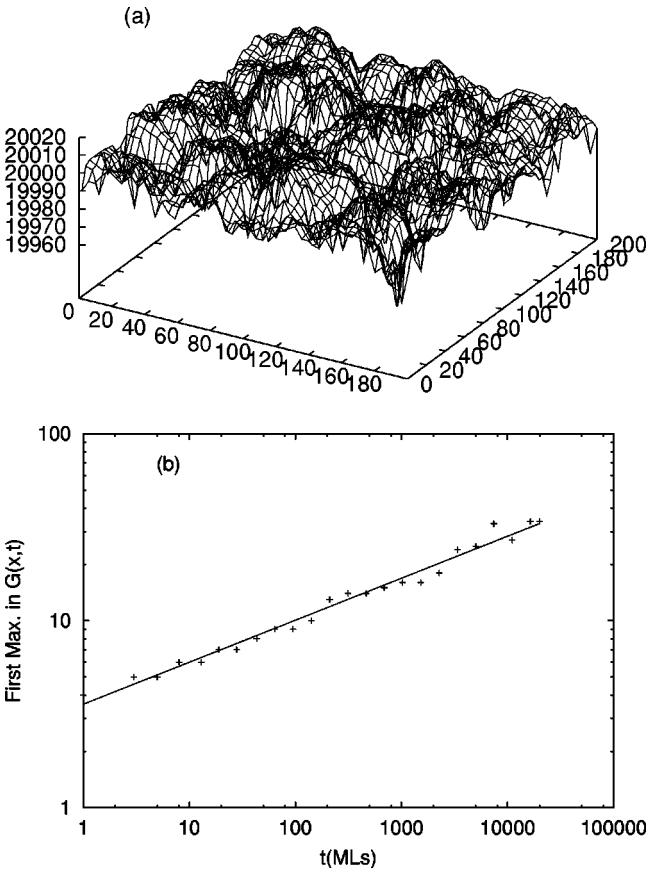

FIG. 3. The growth model with small positive SE barrier but without edge diffusion. The growth is over 200×200 substrate size with SE barrier parameter $p=0.54$ showing small positive barrier to compensate for the larger number of configurations, available for downward hops. (a) Morphology of the surface after 2000 number of layers. (b) Plot of measure of mound size as a function of time. The slope obtained is 0.23 ± 0.02.

B. Effect of dissociation

Contribution to the current from the process of dissociation is obtained as follows. We note that dissociation of freshly deposited adatom will contribute to the nonequilibrium current. Thus, the adatoms deposited at the kink sites or at the bottom of a step with step height more than one are the potential adatoms contributing to the current. Again the density of such sites is $|m|/(1+|m|)$. The flux in this case is c_2F, where c_2 is the fractional flux of adatoms depositing at the potential sites. Let p_d be the probability of dissociation leading to a downward hop. Since steps develop in the direction of the slope, the dissociation current will be downhill current. Thus, a term of the form $-\hat{\mathbf{n}}c'F|m|/(1+|m|)$ is obtained, where c' absorbs all the constants. Expression for this current shows that it does not decrease with m. The uphill current due to the positive SE barrier, and/or edge diffusion is compensated by this current with increasing average local slopes leading to the zero tilt current. Under this condition, the analysis in Sec. IV A applies. To illustrate this point, in our (1+1)-dimensional model, we introduce SE barrier by assigning $p=0.7$. In order to simulate the dissociation effect, we take $q=0.01$. In other words, whenever in the process of diffusion or after the deposition, an adatom with single in-plane neighbor is encountered, it is allowed to dissociate with a probability of 0.01. The dissociated adatom will hop on the terrace or downward across the step depending on the subsequent sequence of random hops. The results are displayed in Figs. 4(a) and 4(b) showing morphology and roughness evolution, respectively. For the sake of comparison, plots corresponding to $q=0.0$ are also included. As seen from Fig. 4(b), the β value for $q=0.01$ is same as the one for the growth with zero tilt current within statistical error. β for $q=0.0$ increases to 1/2 showing instability. The argument is true for higher dimension as well. However, present model is not designed to account the effect of detailed balance. Thus, a stable condition to maintain the TI current is difficult to achieve in our model. In (1+1) dimensions, $n_n=0\leftrightarrow n_n=1$ and $n_n=1\leftrightarrow n_n=1$ are the main processes during surface equilibration. Hence, arriving at the TI current is possible in (1+1) dimensions with our model that includes these processes, controlled through parameters p and q. In (2+1) dimensions, the attachment-detachment processes are many

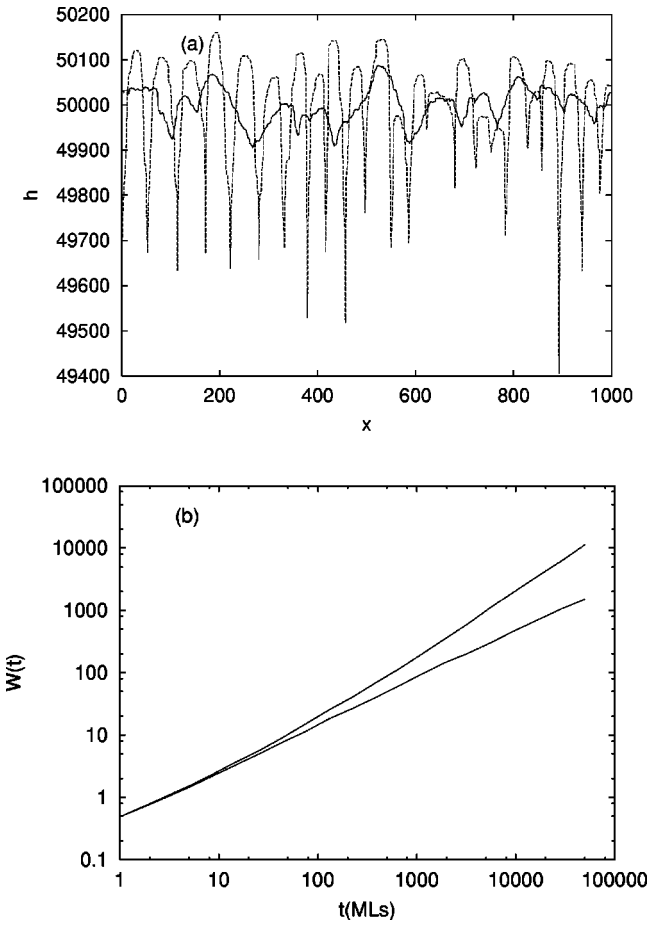

FIG. 4. Comparison of growth model results, with and without dissociation, in $(1+1)$ dimensions. Parameter q decides the fraction of adatoms with single neighbor dissociated if encountered during hopping. (a) Morphology of the surface after 50 000 number of layers. Dotted curve represents morphology in the absence of dissociation while solid one is in the presence of it. (b) Plot of width as a function of time. The β value with dissociation is 0.377 ± 0.007, while that without dissociation increases to 1/2.

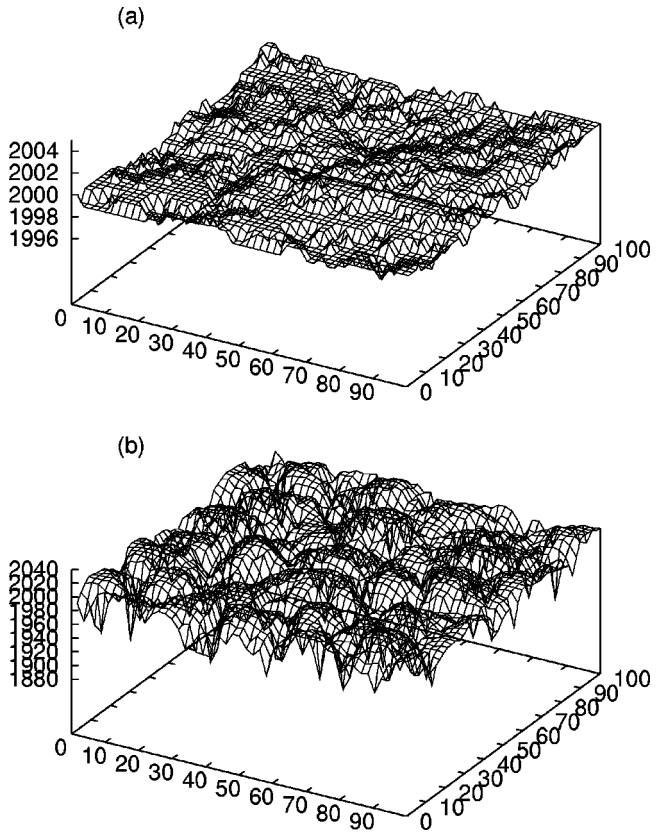

FIG. 5. Comparison of the results for the $(2+1)$-dimensional growth model, with edge diffusion, no diffusion bias ($p=0.5$), and dissociation. Parameter q decides the fraction of adatoms with single neighbor dissociated if encountered during hopping. (a) Morphology of the surface after 2000 number of layers with dissociation ($q=0.4$). Note the absence of mounds in this case. (b) Morphology of the surface after 2000 number of layers without dissociation ($q=0.0$). In this case, mounds grow with $\beta=1/2$.

due to the different possible configurations. Present model does not allow all such processes. Thus, exact tilt independence cannot be attained through the variation of model parameters. Hence, in $(2+1)$ dimensions we illustrate the dissociation effect mainly in the form of stable logarithmic growth. Figures 5(a) and 5(b) show morphology for the case with and without dissociation in $(2+1)$ dimensions, respectively. The effect of dissociation is seen as a stable logarithmic growth compared to the unstable growth with mounding. The surface morphology evolves with $\beta=1/2$ in the latter case. The behavior of $(2+1)$-dimensional model under TI current conditions can be predicted from the form of growth equation. If the steps are straight, then LDV-type term will dominate giving $\alpha=2/3$ and $\beta=1/5$ [16]. However, if mound-like structures are formed, asymmetric term due to the in-plane curvature gradient [Eq. (5)] will be operative leading to $z=4$ and $\beta=1/4$. Siegert and Plischke [34] have considered a symmetric term to explain the pyramidlike structures giving $z=4$ and $\beta=1/4$.

V. GROWTH EQUATIONS FOR OTHER MODELS

A. DT model

As mentioned earlier, the present method for obtaining current from kinetic considerations appropriately brings out the geometrical dependence in growth equation. We have applied this method to the DT model [14], proposed to capture the essential features of low temperature MBE. Based on noise reduction technique, the simulations of this model [32] confirm that (1) exponent $\beta=3/8$ with noise reduction factor unity, while $\beta=1/3$ with noise reduction factor of 10, (2) the morphology is asymmetric with $\sigma\approx-0.5$, (3) the current is TI, and (4) $\alpha=1.4$ and 1.0 with noise reduction factor of unity and 10, respectively [2,32]. The relaxation rules for adatom in this model allow it to hop only when it is deposited at site A or B (see Fig. 1). Also only downward hop is allowed if the adatom is deposited at A and hop toward the step occurs if it is deposited at B. If such favorable configurations are available on two neighboring sites, then it will hop randomly to the left or right. These rules suggest that $P_A=P_B$ for this model. The flux approaching sites A or B in the present set of rules is $F/(a^{-1}+|m|a^{-1})$. For this model, $l_c=a$ since only single hop in definite direction is permitted.

Further, the flux is affected by relative motion of steps only when sites A and B differ by a lattice constant. In Eq. (3), the velocity gradient is considered over the terrace width $(l_c^{-1}+a^{-1}|m|)^{-1}$, which is smaller than l_c. Since the relative motion of steps for above set of rules can affect the flux only for the terrace width of the order of lattice constant a or lower, for the DT model $l_c=a$. As a result of discrete nature of the substrate, further reduction in the terrace width is not possible, this introduces the effect of discretization. Our model, described in Sec. III with $n=1$ and the DT model, is not different in the framework of present analysis. We expect that equation governing the DT model should be applicable to our model. In fact, in our model when local slopes increase in time, the effect of discretization emerges. This effect manifests as a crossover effect where growth exponents during initial growth indicate the LDV-type growth while later it crosses over to the exponents characterizing the DT model, as seen in Sec. IV A. Thus, the current in Eq. (6) with $P_A=P_B$ and including the discretization effect becomes

$$J_{DT}(x)=\nu\frac{\partial^2 m}{\partial x^2}+\frac{\hat{\mathbf{n}}Fa^2}{2}\frac{m}{1+|m|}\partial_x\frac{m}{(1+|m|)^2}. \qquad (8)$$

The growth equation corresponding to this current in the moving frame will be

$$\partial_t h=-\nu\frac{\partial^4 h}{\partial x^4}+\nu_a'\partial_x\frac{m}{1+|m|}\partial_x\frac{m}{(1+|m|)^2}+\eta, \qquad (9)$$

where ν_a' accounts for various constants in the corresponding expression for the current. The power counting in this equation leads to $z=4$ from the first term and $z=1+2\alpha$ for large slopes corresponding to the second term which is expected to be operative mainly over large local inclinations. The relation obtained from the second term is exactly the same as the one obtainable from the noise term η. For $z=4$ all the terms are marginal. This implies that $z=4$ and $\beta=3/8$. The second term breaks the $h\rightarrow -h$ symmetry. Hence, above equation accounts for all the observed facts mentioned above in the simulation of the DT model. Since the growth equation for the DT model is obtained in the discretization limit of surface diffusion model, the surface diffusion model without dissociation approaches DT model asymptotically. Figure 6 shows the plot of W vs time obtained from our $(1+1)$-dimensional model for different values of n. As expected, for $n=1$, β is 3/8. As n increases, it crosses over to this value at later time. Thus, these results clearly demonstrate the effect of discretization in growth.

However, with a large noise reduction factor, the observed behavior of this model corresponds to the LDV-type equation [32]. We have seen that the form of growth equation with large enough terraces is indeed LDV type, as in Eq. (7). The effect of noise reduction technique is to reduce the nucleation noise. In the process, longer terraces are created and *maintained* during growth. Thus, discretization limit is never reached thereby continuing the LDV-type behavior. In both the cases, the current is TI, so the universality of this model

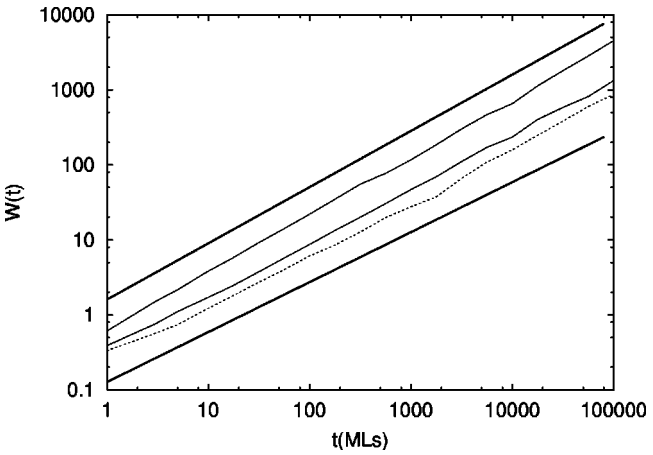

FIG. 6. Plot of width as a function of time for the $(1+1)$-dimensional model described in Sec. III for different number of hops n. Thicker lines with slope of 3/4 and 2/3 are drawn for reference as top curve and bottom curve, respectively. In between, the curves from top correspond to $n=1$, 10, and 25 number of maximum hops. The substrate size is 10000 and SE barrier parameter is 0.5, i.e., no SE barrier.

is ''zero current universality.'' It is a degenerate case since $z=3$ and $z=4$ are both possible for the same model.

In $(2+1)$ dimensions, with above rules for adatom relaxation, the local density of sites A and B need not be equal since fluctuations in step edges render configurations that show bias for sites A or B. As a result, slope dependent current will dominate the growth changing the universality class with dimensions [32]. In this case, the noise reduction technique helps to establish the sign of the current on tilted substrate. Without noise reduction, the nucleation noise obscures the real sign of the current and hence the universality of the model in $(2+1)$ dimensions. In particular, for the DT model, it has been shown that [32] configurations favor downward hops. Thus, in spite of intrinsic randomness in selecting the neighboring site for a hop, a downhill current is produced on tilted substrate leading to Edward-Wilkinson (EW)- [26] type universality.

B. WV model

This model was introduced by Wolf and Villain [15] to simulate low temperature MBE growth. In this model, relaxation rules require that an adatom will hop to a nearest site if n_n increases. Thus, for hops from $n_n=0\rightarrow n_n=1$, the model is same as the DT model. However, it allows hops from $n_n=1\rightarrow n_n=2$ that cause adatoms to dissociate from steps and hop *into* the surface. Thus it is closer that, WV model will follow the DT model equation above. In addition, due to the dissociation, downhill current is produced as has been discussed in Sec. IV B. The current on tilted substrate has been measured for this model and is confirmed to be downhill [35].

In $(2+1)$ dimensions, hops from smaller n_n to higher n_n imply edge diffusion. This can compensate the dissociation induced downhill current. Das Sarma *et al.* [32] have observed mound formation in $(2+1)$-dimensional WV model.

C. LD Model

This model was introduced by Lai–Das Sarma [16] in connection with the LDV equation. The rules were set based on the geometric interpretation of the term $\nabla^2(\nabla h)^2$. Accordingly, a zero neighbor adatom follows same rules as depicted for the DT model. If the adatom is deposited at a kink site with a single lateral nearest neighbor, it is allowed to move to the nearest kink site with smaller step height. Thus, an upward or downward hop is permitted to satisfy the rule. The rule suggests that a hop from one kink site to the neighboring one is allowed from *smaller to larger local slope*. Thus, flux in expression (1) is $c_l F(m/|m|)(\partial m/\partial x)$, where c_l is the fraction of the incident flux F, landing at kink sites. The factor $m/|m|$ ensures proper direction. The probability for hopping, once the appropriate configuration is attained, is unity as per the relaxation rules for the model. From Eq. (1), the term in the growth equation due to the kink to kink hopping is

$$\partial_x\left(c_l F \frac{m|m|}{|m|(1+|m|)} \frac{\partial m}{\partial x}\right).$$

This term is consistent with the requirement of invariance under $x\rightarrow -x$. For small m, it reduces to $(\partial^2/\partial x^2)(\partial h/\partial x)^2$. However, this term is expected to contribute mainly for larger slopes when the steps with terraces of unit length appearing consecutively are large enough in number. Under these conditions, the term reduces to $\partial_x((m/|m|)(\partial m/\partial x))$. This term under scaling hypothesis, $x\rightarrow bx$ and $t\rightarrow b^z t$ gives exponent $z-3$. If this term is not renormalized, it leads to the same scaling exponents as given by $(\partial^2/\partial x^2)(\partial h/\partial x)^2$, i.e., $z=3$, $\alpha=1$, and $\beta=1/3$.

VI. DISCUSSION

Our results show that a growth situation where kinetics of adatoms is well defined can be understood using proposed methodology for obtaining the growth equation. It is therefore perfectly suited for computer models with well defined relaxation rules.

The results indicate that in real MBE growth, within a low temperature range where evaporation is still negligible, one can expect different behavior for different materials on a singular surface. The activation barriers for hopping across an edge (SE barrier), edge diffusion, and dissociation are expected to be in the ascending order. As the temperature increases, the corresponding processes are expected to be activated in the same order. Thus, for materials with very small or zero SE barrier, at low temperatures TI current will dictate the morphology evolution. In many cases, it will be with $z=4$ and $\beta=1/4$. At higher temperature, edge diffusion is activated causing instability. This will lead to $\beta=1/2$ asymptotically. At higher temperatures, dissociation will reduce the uphill current to TI current. However, this situation has to compete with the step flow that leads to EW-type growth [20]. This scenario is well fitted to the growth of Cu [36]. If the SE barrier is high, at low temperature, unstable growth will appear with $\beta=1/2$ [37]. At higher temperature, edge diffusion will not change the exponent. But once the dissociation is activated, TI current will reduce β. In this study, we have neglected effects of upward hops. These can further add more scenarios [12]. It has been mentioned [12] that with in-plane hops, β cannot exceed the value 1/2. The transients in the growth are, however, known to produce higher apparent values of β [2]. Also, upward hops can give a value as high as 1 for β [12].

So far, we have focused our discussion in the vicinity of the TI current. We can gain a better insight into the growth behavior by applying the above method for the analysis of the growth with uphill current. Above arguments suggest that the growth equation that we have obtained is specific to the stepped region on the surface. From the kinetics of adatoms on top or base terraces, it is clear that the growth equation can be different in these regions [17]. This will lead to the breakdown of spatial invariance. We argue that regions that allow restricted types of kinetics will support fewer terms in the growth equation than the ones that allow larger number of kinetic processes. We will examine the scenario in $(1+1)$ dimensions, however, the argument is easily extended in $(2+1)$ dimensions. By inspection, we can identify three regions that allow different number of kinetic processes, (1) a top terrace, defined between two down going step edges, (2) a base region, defined between two up going step edges, and (3) stepped regions, are three distinct regions. On time scales $\ll \tau_{ML}$, a stepped region allows downward hops, relative step motion, and in-plane hops. Thus, the growth equation corresponding to the current in Eq. (6) , including all the three terms is valid over this region. The top terrace in the absence of nucleation allows downward hops. By symmetry, the current must be TI, so that it will support only Mullin's term. On the base region, only in-plane hops are possible. Again by symmetry the current must be TI. In this region only Poisson-type growth with no apparent term to build the h-h correlations is allowed. In order that such a description is valid on reasonable time scales, it is necessary that these regions maintain their identity over appreciable time. The corresponding time should be at least τ_{ML}, which is the minimum time for a height fluctuation at a given site. Accordingly, if a base region is created locally, then its dwelling time at the given place decides whether it will act as an independent region or not. In order to get a qualitative idea of stability of base regions over time, we have performed simulations of an isolated base region as depicted in Figs. 7(a) and 7(b). We grow few layers allowing dynamics of adatoms as per the growth model described in Sec. III and compute the time correlations for height. The correlations are obtained at different values of the model parameter p while keeping $q=0$. The width of the base region is of the order of diffusion length. The number of hops n are chosen accordingly. We have also employed noise reduction technique to reduce the nucleation noise. Figures 7(a) and 7(b) show typical development of base region for the parameter $p=0.1$ and 0.9, respectively. Figure 7(c) shows the time correlations $G_t(\tau)=\langle h(x,0)h(x,\tau)\rangle$, for various values of p. The base region in real growth can occur in various surrounding configurations. Although stability times of such configuration will differ, the trend depicted in Fig. 7(c) is observed to apply to them. The nature of these plots shows that (a) the

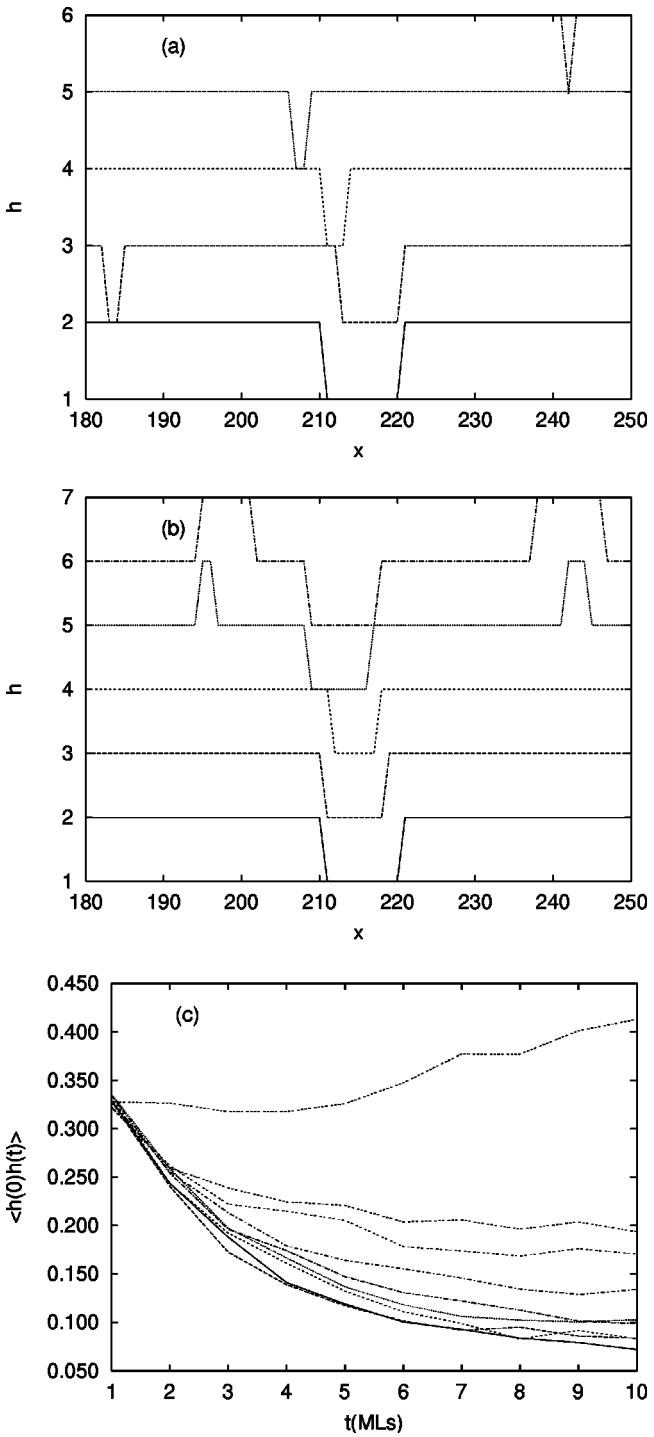

FIG. 7. (a) Time development of a base region of width 10 units, bounded by single steps of unit height. Figure shows the morphology for four layers grown with the parameter $p=0.1$ and $n=100$ for the model described in Sec. III. (b) Time development of the base region for ML as in (a), but the model parameter $p=0.9$ implying large SE barrier. The base region is seen to be stable in this case. (c) Plot of time correlation function $\langle h(0)h(t)\rangle$ for the growth over base region depicted in (a) and (b). The topmost curve corresponds to the model parameter value $p=0.9$ while curves corresponding to $p=0.8$, 0.7, 0.6, 0.5, 0.4, 0.3, 0.2, and 0.1 appear below it in the descending order.

characteristic time τ_b for the decay depends on p such that, τ_b increases with p, and (b) for $p=0.9$, $\tau_b\to\infty$. Observation (b) is important to us. We find that as long as $p>0.5$ (i.e., *current is uphill*), there is a threshold for the depth of the base region, beyond which $\tau_b\to\infty$. For $p=0.9$ this happens for a single-step depth. In such a region, there are no kinetic processes that can support growth of h-h correlations in the vicinity. Since no correlations can be built in this region, it reduces in size. It acts as a discontinuous region with respect to the adjoining stepped regions. Corresponding simulations under these conditions will always result in the formation of deep ridges. This discussion suggests that, whenever $p\neq 0$, initially, there will be regions on the substrate during growth separated by local base regions. However, as long as base region decays in time with finite τ_b, the lateral growth of h-h correlations continues as per the growth equation on stepped region. In this sense, the growth equation is valid over the entire substrate. As growth proceeds, deeper base regions will be created by fluctuations. If these base regions do not decay in time, which is always the case when current on tilted substrate is uphill, ridges are formed. Lateral growth of the regions separated by a ridge is then governed by the dynamics of adatoms across the ridge and *not by the growth equation on the stepped region*. Thus, the continuum equation approach fails to describe the growth in such cases. As a result, in $(1+1)$ dimensions, the mounds grow as $\ln(t)$ asymptotically. In $(2+1)$ dimensions the mound growth is slower than $\ln(t)$. Power law dependence in time is observed *only for TI current and downhill current growth* [17].

In Sec. II, we have discussed growth under infinite SE barrier. Above proposition of the disconnected substrate under uphill current is consistent with the observed symmetric growth for infinite SE barrier in $(1+1)$ dimensions [23]. For the model, growth in $(1+1)$ dimensions with the rules in Sec. III, unstable growth occurs for $1.0>p>0.5$ rendering uphill current. For such growth according to the previous analysis, the base region supports only Poisson-type growth while the top region can generate $\partial^4 h/\partial x^4$ term. Therefore, the top regions are flat while base regions have sharp ridges breaking $h\to -h$ symmetry. However, for infinite SE barrier, i.e., for $p=1.0$, top region cannot generate fourth-order smoothening term due to the absence of downward hops. Thus, both base and top regions support only Poisson growth rendering symmetric pattern.

VII. CONCLUSION

In conclusion, we have proposed a simple method for obtaining current in a solid-on-solid growth in $(1+1)$ dimensions. The resultant growth equation shows that the presence of diffusion alone is responsible for roughening of a singular surface. It induces an asymmetric term in the continuum equation. The velocity gradient of steps on a growing surface is responsible for such a term. In $(2+1)$ dimensions, in-plane curvature gradient generates an asymmetric term. This term is responsible for asymmetry in the growth on a two-dimensional substrate with infinite SE barrier. Role of in-plane hops is seen to smoothen out the deposition noise in a plane, within diffusion length. The corresponding terms gen-

erated are operative only within the plane. A curvature dependent term is seen to arise from downward hops. Study of zero bias model brings out effects of discretization and violation of detailed balance. A stable→unstable transition with symmetry breaking results from such a violation. In this context, the present study brings out the effect of dissociation on the asymptotic behavior of growth. In the absence of upward hops, dissociation introduces a downhill current. The condition of detailed balance requires dissociation as a part of the process toward equilibration. Thus, at high enough temperatures, a zero tilt current is expected to dictate the growth morphology. Considering the processes in a KMC simulation, it is conjectured that these simulations are close to TI current even when SE barriers are included in simulations. The method is successfully applied to various models in the literature. It provides an insight into the role of kinetics in the growth from vapor. In the DT model, in particular, it supports the dimensional dependence of universality class for growth under DT rules. The continuum equation approach is, however, seen to be restricted to zero or downhill current on tilted substrates. For uphill current, disjoint regions following different growth equations are obtained.

ACKNOWLEDGMENT

The author acknowledges useful suggestions by Professor S. Das Sarma, University of Maryland, College Park, Maryland, U.S.A.

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