Growth equations for the Wolf-Villain and Das Sarma–Tamborenea models of molecular-beam epitaxy

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We derive the growth equations for the Wolf-Villain and Das Sarma–Tamborenea models based on the master-equation method. The Wolf-Villain model is shown to obey the conserved growth equation $\partial h/\partial t = -\nu_4 \nabla^4 h + \lambda_{22}\nabla^2(\nabla h)^2 + \Sigma_{n=1}^{\infty}\lambda_{12n+1}\nabla\cdot(\nabla h)^{2n+1} + F + \eta$, which is expected to exhibit the scaling behavior of the Edwards-Wilkinson universality class. We find that the Das Sarma–Tamborenea model is governed by the Villain–Lai–Das Sarma equation $\partial h/\partial t = -\nu_4\nabla^4 h + \lambda_{22}\nabla^2(\nabla h)^2 + F + \eta$ in contrast to former results. The physical origin of the difference between these two similar models is also discussed. [S1063-651X(96)00611-3]

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I. INTRODUCTION

Kinetic roughening of nonequilibrium surface growth has been of great interest in recent years. The kinetic growth processes have been intensively studied via various discrete models and continuum equations and exhibit nontrivial scaling behavior [1,2]. The surface width W, which is the root-mean-square fluctuation of the surface height, scales as $W(L,t) \sim L^{\alpha} f(t/L^z)$, where the scaling function $f(x)$ is constant for $x \gg 1$ and x^{β} for $x \ll 1$ with $\beta = \alpha/z$. The scaling behaviors of the growth are characterized by the roughness exponent α, the growth exponent β, and the dynamical exponent z, and these exponents determine the universality class.

Recently, much attention has been paid to the surface growth via molecular-beam epitaxy (MBE) [3–11]. The conserved growth conditions are applied in the idealized MBE without both defect and evaporation, and there are many discrete models [3–8] describing this type of growth process. The simulations using these discrete models are carried out according to the given growth rules that govern the physical properties of surface growth. Among a large number of growth models, two similar microscopic models proposed, respectively, by Wolf and Villain [5] and Das Sarma and Tamborenea [6] have attracted much interest. Instead of moving to the local height minimum, the deposited particles relax into sites maximizing the coordination numbers in the Wolf-Villain (WV) model or to neighboring kink sites in the Das Sarma–Tamborenea (DT) model, respectively. In the early simulations [5,6], the two models were shown to be within the same universality class and follow the Herring-Mullins linear diffusion equation [12]

$$\frac{\partial h}{\partial t} = -\nu_4 \nabla^4 h + \eta, \tag{1}$$

where $h(\mathbf{x},t)$ is the height of the surface at time t in $d = d' + 1$ dimensions, d' is the substrate dimension, $\mathbf{x}$ is d'-dimensional vector, and η is the nonconserved Gaussian white noise.

However, numbers of recent extensive studies [4,13–17] cast doubt on the original results and suggested that these two diffusion models actually belong to different universality classes in spite of their apparent similarities. Much more attention has been focused on the WV model. Some numerical simulations [4,13] have shown that in 2+1 dimensions the WV model corresponds to the Villain–Lai–Das Sarma (VLD) equation [9,10] with the relevant $\nabla^2(\nabla h)^2$ nonlinearity. But a detailed analysis based on the study of surface diffusion current [14] and computer simulations [15] revealed that the WV model asymptotically belongs to the Edwards-Wilkinson (EW) universality class [18] corresponding to a continuum differential equation with the $\nabla^2 h$ EW term. More recently, crossover behavior in the WV model has been observed in both 1+1 and 2+1 dimensions [16,17]. Extensive computer simulation was carried out by Šmilauer and Kotrla [16] to show the crossover from the scaling behavior of linear equation (1) to the VLD behavior and finally the crossover to the EW class. Moreover, according to a natural extension of the WV model within the next-nearest-neighbor approximation, which leads to no change of the main results, Ryu and Kim [17] observed the crossover effect from the VLD behavior to the EW class in a clearer manner. In these studies [16,17], the WV model is thought to be governed by a continuum growth equation with the existence of the $\nabla^2 h$ EW term, which is more relevant than all other nonlinear terms and determines the asymptotic behavior of the model.

It has been found by studying the height-height correlation function and the structure factor [19] that the DT model obeys anomalous dynamic scaling. A similar result has been presented for the WV model [20,16]. Recently, it has been suggested by Krug [21] that in the absence of tilt invariance the DT model may be described by a continuum growth equation with an infinite sequence of relevant terms $\lambda_{22}\nabla^2(\nabla h)^2 + \lambda_{24}\nabla^2(\nabla h)^4 + \cdots$, which is just the VLD equation if only the first nonlinearity is kept. Halpin-Healy and Zhang [2] also estimated that the DT model results in the asymptotic behavior that most likely will be VLD based on the analysis of the tilt-dependent surface current proposed by

Krug, Plischke, and Siegert [14]. But to our knowledge, these suggestions have not been verified by numerical simulation or analytical deduction.

There have been several attempts to establish the equivalence between the discrete growth models and corresponding continuum growth equations [3–10]. Most of the work is done numerically by comparing the simulated exponents of the discrete models with those of the continuum equations. There are also some analytic studies to establish the connection [22–26]. Beginning with the master-equation description, Vvedensky *et al.* [22,23] proposed a systematic method to derive the continuum equations from growth rules of the discrete models. Originally, this method was introduced for the Arrhenius-type surface processes [22,23], and recently it has been successfully applied [24] to deriving the Kardar-Parisi-Zhang equation [27] from the restricted solid-on-solid (RSOS) model [28].

In this work we investigate the WV and DT models by deriving their corresponding growth equations in 1+1 dimensions based on the method of Vvedensky *et al.* [22,23]. For the WV model, the EW term ($\nabla^2 h$) does not exist; instead, the continuum growth equation becomes

$$\frac{\partial h}{\partial t}=-\nu_4\nabla^4 h+\lambda_{22}\nabla^2(\nabla h)^2+\sum_{n=1}^{\infty}\lambda_{12n+1}\nabla\cdot(\nabla h)^{2n+1}+F+\eta, \qquad (2)$$

where ν_4, λ_{22}, and λ_{12n+1} are growth coefficients and F is the deposition flux. According to the conclusion of both the direct numerical integration [29] and the dynamical renormalization-group (DRG) analysis [30,31], the relevant $\nabla\cdot(\nabla h)^{2n+1}$ term in Eq. (2) is verified to produce the scaling properties of the EW class if λ_{12n+1} is positive. However, we obtain that $\lambda_{13}<0$, $\lambda_{15}>0$, $\lambda_{17}<0$, $\lambda_{19}>0,\ldots$, that is, the coefficients λ_{12n+1} are negative and positive alternatively. In 1+1 dimensions, we expect Eq. (2) to obey the EW asymptotic behavior according to some phenomenological analyses, although further extensive studies are needed. We also find that the DT model is governed by the VLD equation

$$\frac{\partial h}{\partial t}=-\nu_4\nabla^4 h+\lambda_{22}\nabla^2(\nabla h)^2+F+\eta, \qquad (3)$$

which is inconsistent with the previous numerical simulations [6,4,19], but confirms the estimation of Halpin-Healy and Zhang [2].

In Secs. II and III we show the derivation of the growth equations for the WV model and the DT model, respectively. The discussion and conclusion are presented in Sec. IV.

II. GROWTH EQUATION FOR THE WOLF-VILLAIN MODEL

The derivation process in the method of Vvedensky *et al.* [22,23] begins with the master-equation description of the microscopic dynamics of the discrete model. With the given transition rates between configurations of the lattice, the nonlinear discrete Langevin equation and its associated noise covariance can be obtained. Subsequently, a nonrigorous regularization procedure is introduced to pass to the continuum limit and the continuum stochastic equation is directly derived. Here we use the method for one-dimensional substrate growth [22] to derive the continuum growth equation for the WV model, and the generalization to higher dimensions is straightforward [23].

First, we specify the configuration of the surface by $\mathbf{H}=\{h_1,h_2,\ldots\}$, where h_i, $i=1,2,\ldots$, are the column height variables. The evolution of the joint probability distribution $P(\mathbf{H};t)$ is determined by a birth-death-type master equation

$$\frac{\partial P(\mathbf{H};t)}{\partial t}=\sum_{\mathbf{H}'}W(\mathbf{H}',\mathbf{H})P(\mathbf{H}';t)-\sum_{\mathbf{H}'}W(\mathbf{H},\mathbf{H}')P(\mathbf{H};t), \qquad (4)$$

where $W(\mathbf{H},\mathbf{H}')$ is the transition rate from the configuration $\mathbf{H}$ to the configuration $\mathbf{H}'$ and reflects the microscopic process of the discrete model.

The above master equation can be turned into the Kramers-Moyal form [32] with the transition moments of $W(\mathbf{H},\mathbf{H}')$. In the limit of large system size, it has been shown by Fox and Keizer [33] that only the first and second transition moments

$$K_i^{(1)}=\sum_{\mathbf{H}'}(h_i'-h_i)W(\mathbf{H},\mathbf{H}'), \qquad (5)$$

and

$$K_{ij}^{(2)}=\sum_{\mathbf{H}'}(h_i'-h_i)(h_j'-h_j)W(\mathbf{H},\mathbf{H}'), \qquad (6)$$

are required, and the Kramers-Moyal form reduces to the Fokker-Planck equation

$$\frac{\partial P(\mathbf{H};t)}{\partial t}=-\frac{\partial}{\partial h_i}[K_i^{(1)}P(\mathbf{H};t)]+\frac{1}{2}\frac{\partial^2}{\partial h_i\partial h_j}[K_{ij}^{(2)}P(\mathbf{H};t)], \qquad (7)$$

which is equivalent to the Langevin equation

$$\frac{dh_i}{dt}=K_i^{(1)}+\eta_i(t). \qquad (8)$$

The Gaussian white noise η_i in Eq. (8) satisfies

$$\langle\eta_i(t)\rangle=0, \qquad (9)$$

$$\langle\eta_i(t)\eta_j(t')\rangle=K_{ij}^{(2)}\delta(t-t'). \qquad (10)$$

In previous work, the Langevin equation (8) was obtained on the condition that the intrinsic fluctuations are not too large [22,24]. When the intrinsic fluctuations grow large and consequently the distribution $P(\mathbf{H};t)$ becomes broad, we can make use of a limit theorem of Kurtz [34] to handle the large intrinsic fluctuations. Therefore, as shown by Fox and Keizer [33], the Kurtz limit theorem produces the Fokker-Planck equation (7), which is equivalent to Eq. (8) in the Itô version of stochastic calculus. Thus, for the MBE growth models such as the WV and DT models, where the surfaces are very rough and the step height distribution spreads out [20,21], the Langevin equation (8) can determine the growth dynamics of the models and give a description of the rough growth surfaces. Therefore, to obtain the explicit form of the discrete Langevin equations and the noise covariance, we should determine the quantity $W(\mathbf{H},\mathbf{H}')$ according to the growth rule of the specific discrete model and, subsequently, the transition moments $K_i^{(1)}$ and $K_{ij}^{(2)}$ using Eqs. (5) and (6).

In the WV model [5], a particle is deposited onto the substrate randomly and is allowed to relax into the surface site with the strongest binding, i.e., the largest coordination numbers. If more than one neighboring site is equally preferable, one of them is chosen at random. During the growth process, if a particle sticks on one site i, $h_i \to h_i + a$, where a is the lattice constant. We suppose that the average deposition time for a layer is τ and the configuration of the lattice is changed via random deposition at an average rate of τ^{-1}. Therefore, the transition rate is written as

$$W(\mathbf{H},\mathbf{H}') = \tau^{-1}\sum_k \left[w_k^{(1)}\delta(h_k', h_k + a)\prod_{j\neq k}\delta(h_j', h_j) + w_k^{(2)}\delta(h_{k-1}', h_{k-1}+a)\prod_{j\neq k-1}\delta(h_j', h_j) + w_k^{(3)}\delta(h_{k+1}', h_{k+1}+a)\prod_{j\neq k+1}\delta(h_j', h_j)\right], \tag{11}$$

where

$$\begin{aligned} w_k^{(1)} = {} & \Theta(h_{k-1}-h_{k-2})\Theta(h_{k+1}-h_{k+2})\delta(h_{k-1},h_k) \\ & \times\delta(h_{k+1},h_k) + \Theta(h_{k-1}-h_k)\Theta(h_{k+1}-h_k) - \delta(h_{k-1},h_k)\delta(h_{k+1},h_k) + [1-\Theta(h_k-h_{k-1})] \\ & \times[1-\Theta(h_{k+1}-h_k)]\Theta(h_{k+1}-h_{k+2}) + \Theta(h_{k-1}-h_{k-2})[1-\Theta(h_{k-1}-h_k)] \\ & \times[1-\Theta(h_k-h_{k+1})], \end{aligned} \tag{12}$$

$$\begin{aligned} w_k^{(2)} = {} & \delta(h_{k-1},h_k)\delta(h_k,h_{k+1})[1-\Theta(h_{k-1}-h_{k-2})] \\ & \times(\Theta(h_{k+1}-h_{k+2}) + \tfrac{1}{2}[1-\Theta(h_{k+1}-h_{k+2})]) \\ & + \delta(h_k,h_{k+1})[1-\Theta(h_{k-1}-h_k)][\Theta(h_{k+1}-h_{k+2}) \\ & + [1-\Theta(h_{k+1}-h_{k+2})]([1-\Theta(h_{k-1}-h_{k-2})] + \tfrac{1}{2}\Theta(h_{k-1}-h_{k-2}))] \\ & + \tfrac{1}{2}\,\delta(h_{k-1},h_k)[1-\Theta(h_{k+1}-h_k)][1-\Theta(h_{k-1}-h_{k-2})]\Theta(h_{k+1}-h_{k+2}) \\ & + [1-\Theta(h_{k-1}-h_k)][1-\Theta(h_{k+1}-h_k)]([1-\Theta(h_{k-1}-h_{k-2})]\Theta(h_{k+1}-h_{k+2}) + \tfrac{1}{2}\{\Theta(h_{k-1}-h_{k-2})\Theta(h_{k+1}-h_{k+2}) \\ & + [1-\Theta(h_{k-1}-h_{k-2})][1-\Theta(h_{k+1}-h_{k+2})]\}) + [1-\Theta(h_{k-1}-h_{k-2})][1-\Theta(h_{k-1}-h_k)][1-\Theta(h_k-h_{k+1})], \end{aligned} \tag{13}$$

and

$$\begin{aligned} w_k^{(3)} = {} & \delta(h_{k-1},h_k)\delta(h_k,h_{k+1})[1-\Theta(h_{k+1}-h_{k+2})](\Theta(h_{k-1}-h_{k-2}) + \tfrac{1}{2}[1-\Theta(h_{k-1}-h_{k-2})]) \\ & + \tfrac{1}{2}\,\delta(h_k,h_{k+1})[1-\Theta(h_{k-1}-h_k)][1-\Theta(h_{k+1}-h_{k+2})]\Theta(h_{k-1}-h_{k-2}) + \delta(h_{k-1},h_k)[1-\Theta(h_{k+1}-h_k)] \\ & \times[\Theta(h_{k-1}-h_{k-2}) + [1-\Theta(h_{k-1}-h_{k-2})]([1-\Theta(h_{k+1}-h_{k+2})] + \tfrac{1}{2}\Theta(h_{k+1}-h_{k+2}))] \\ & + [1-\Theta(h_{k-1}-h_k)][1-\Theta(h_{k+1}-h_k)](\{\Theta(h_{k-1}-h_{k-2})[1-\Theta(h_{k+1}-h_{k+2})] \\ & + \tfrac{1}{2}\{\Theta(h_{k-1}-h_{k-2})\Theta(h_{k+1}-h_{k+2}) + [1-\Theta(h_{k-1}-h_{k-2})][1-\Theta(h_{k+1}-h_{k+2})]\}) \\ & + [1-\Theta(h_k-h_{k-1})][1-\Theta(h_{k+1}-h_k)][1-\Theta(h_{k+1}-h_{k+2})]. \end{aligned} \tag{14}$$

The $w_k^{(1)}$ term presents the situation that a particle is deposited at site k and stays there, while the $w_k^{(2)}$ and $w_k^{(3)}$ terms describe the processes that the deposited particle at site k hops to the nearest sites $k-1$ or $k+1$, respectively. $\Theta(x)$ in these formulas is the unit step function defined by

$$\Theta(x)=\begin{cases}1 & \text{if } x\geqslant 0\\ 0 & \text{if } x<0.\end{cases} \tag{15}$$

From Eqs. (12)–(14) we obtain the identity

$$w_k^{(1)}+w_k^{(2)}+w_k^{(3)}=1, \tag{16}$$

which guarantees that the average deposition rate per site remains τ^{-1}. From Eqs. (5) and (6), the first and second transition moments become

$$K_i^{(1)}=\frac{a}{\tau}[w_i^{(1)}+w_{i+1}^{(2)}+w_{i-1}^{(3)}], \tag{17}$$

$$K_{ij}^{(2)}=aK_i^{(1)}\delta_{ij}. \tag{18}$$

It is noted that formulas (16)–(18) are similar to those of hot-atom effects discussed by Vvedensky *et al.* [22]. Thus, using Eqs. (8)–(10), we can obtain the discrete Langevin equation for the WV model.

Next, presuming that the discrete height variable of the surface $h_i(t)$ can be replaced by a analytic function $h(x,t)$, we regularize the discrete Langevin equation by expanding the nonanalytic quantities and replacing them with analytic quantities. First, the step function can be approximated by an analytic shifted hyperbolic tangent function and expanded in a Taylor series [22,24]

$$\Theta(x)\approx 1+\sum_{k=1}^{\infty} A_k x^k. \tag{19}$$

Then taking the limit of lattice constant $a\to 0$, we expand $(h_{i\pm 1}-h_i)$, $(h_{i\pm 2}-h_{i\pm 1})$, etc., in powers of a, and replace $h_i(t)$ by a function $h(x,t)$ with $x=ia$ that is smooth at the macroscopic scale. During the derivation, we also note the relation

$$\delta(h_i,h_j)=\Theta(h_i-h_j)+\Theta(h_j-h_i)-1 \tag{20}$$

according to the definition (15) of the step function. Therefore, substituting (12)–(14) into (17) and (18), and expanding up to $O(a^5)$, after simple but tedious deduction the transition moments are obtained as

$$\begin{aligned}K^{(1)}(x)&=\frac{a}{\tau}\left\{1-A_1a^4\frac{\partial^4 h}{\partial x^4}+2(-A_1^2+2A_2)a^4\left[\left(\frac{\partial^2 h}{\partial x^2}\right)^2+\left(\frac{\partial h}{\partial x}\right)\left(\frac{\partial^3 h}{\partial x^3}\right)\right]-6A_1^3a^4\left(\frac{\partial h}{\partial x}\right)^2\left(\frac{\partial^2 h}{\partial x^2}\right)\right\}+O(a^6)\\ &=\frac{a}{\tau}\left[1-A_1a^4\frac{\partial^4 h}{\partial x^4}+(-A_1^2+2A_2)a^4\frac{\partial^2}{\partial x^2}\left(\frac{\partial h}{\partial x}\right)^2-2A_1^3a^4\frac{\partial}{\partial x}\left(\frac{\partial h}{\partial x}\right)^3\right]+O(a^6)\end{aligned} \tag{21}$$

and

$$K^{(2)}(x,x')=\frac{a^2}{\tau}\delta(x-x')+O(a^6). \tag{22}$$

From Eq. (8), the continuum growth equation for the WV model is just described by Eq. (2) with only the first term $n=1$ in the infinite series, that is,

$$\frac{\partial h}{\partial t}=-\nu_4\nabla^4 h+\lambda_{22}\nabla^2(\nabla h)^2+\lambda_{13}\nabla\cdot(\nabla h)^3+F+\eta, \tag{23}$$

and the coefficients are given by

$$\nu_4=\frac{a^5}{\tau}A_1,$$

$$\lambda_{22}=\frac{a^5}{\tau}(-A_1^2+2A_2),$$

$$\lambda_{13}=-\frac{2a^5}{\tau}A_1^3,$$

$$F=\frac{a}{\tau}. \tag{24}$$

The noise covariance given in Eq. (10) is

$$\langle\eta(x,t)\eta(x',t')\rangle=\frac{a^2}{\tau}\delta(x-x')\delta(t-t'). \tag{25}$$

Since the unit step function is approximated by the shifted hyperbolic tangent function and $\tanh x\sim x-x^3/3+2x^5/15-17x^7/315+\cdots$, we have $A_1>0$, $A_3<0$, $A_5>0$, $A_7<0,\ldots$ and A_2, A_4, $A_6,\ldots$ are very small and negligible in Eq. (19). Therefore, from Eq. (24), we obtain that $\nu_4>0$, which is consistent with the phenomenological consideration $\lambda_{22}<0$ and $\lambda_{13}<0$.

The fourth-order conserved growth equation (23) was proposed by Lai and Das Sarma [10], and $\nabla\cdot(\nabla h)^3$ nonlinearity is the most relevant term from the renormalization-group viewpoint. Although there is no EW term in Eq. (23), the direct numerical integration study [29] and the one-loop DRG calculation [30] showed that for positive λ_{13} the calculated exponents are consistent with those of the EW universality class in 1+1 dimensions. However, the coefficient λ_{13} we derive is negative, which gives rise to unstable surface growth. This result of instability is surprising and contradicts the results of numerical simulations [15–17] and the analysis of surface diffusion current [14]. Thus we expand $K_i^{(1)}$ to higher orders. We find that the terms of $O(a^{2n})$ for $K_i^{(1)}$ [i.e., the odd order of a, $O(a^{2n-1})$, for $w_i^{(1)}+w_{i+1}^{(2)}+w_{i-1}^{(3)}$] vanish, which is due to the symmetry between sites $i+n$ and $i-n$ in the surface, that is, the consideration of isotropic surface growth in the model. The terms appearing in the growth equation are $(m,n\geqslant 1)$ the linear terms $\nabla^{2n+2}h$, the nonlinearities $\nabla^{2m-1}\cdot(\nabla h)^{2n+1}$, which generate terms $\nabla^{2m-2}\nabla^2 h$ according to the DRG analysis by Kshirsagar and Ghaisas [31], and the nonlinearities $\nabla^{2m}(\nabla h)^{2n}$, which generate terms $\nabla^{2m}(\nabla h)^2$ also according to Kshirsagar and Ghaisas [31]. Among these, the most relevant terms are $\nabla\cdot(\nabla h)^{2n+1}$, which lead to the EW term $\nabla^2 h$ if the corresponding coefficients are positive. Therefore, keeping the meaningful lowest-order terms $\nabla^4 h$ and $\nabla^2(\nabla h)^2$, we obtain the growth equation (2) for the WV model.

We also obtain the explicit forms of coefficients λ_{12n+1} of the relevant nonlinearities $\nabla\cdot(\nabla \mathrm{h})^{2n+1}$: $\lambda_{13}=-2a^5A_1^3/\tau$ as in (24) and $\lambda_{15}=(-6A_1^2A_3-4A_1^3A_2+2A_1A_2^2)a^7/\tau$. In the forms of λ_{17} and λ_{19} there are 7 and 13 terms, respectively, and we show only the leading ones: $\lambda_{17}=(-6A_1^2A_5-6A_1A_3^2+\cdots)a^9/\tau$ and $\lambda_{19}=(-6A_1^2A_7-12A_1A_3A_5-2A_3^3+\cdots)a^{11}/\tau$, where the ellipses represent terms with negligible A_2, A_4, and A_6. From the signs of A_1, A_3, A_5, and A_7 shown above, we have $\lambda_{13}<0$, $\lambda_{15}>0$, $\lambda_{17}<0$, $\lambda_{19}>0,\ldots$.

Thus it is interesting to discuss the properties of Eq. (2) where the coefficients λ_{12n+1} of the relevant terms are negative and positive alternatively. For the WV model only the downhill surface current is generated in 1+1 dimensions, and according to the method of surface diffusion current [14], the WV model is shown to belong to the EW universality class. Therefore, it can be argued that Eq. (2), which describes the WV model, most likely will obey the EW behavior in 1+1 dimensions. A recent work carried out by Kim [35] is instructive, where a discrete model following an equation $\partial h/\partial t=\nu_2\nabla^2 h-\nu_4\nabla^4 h+\lambda_{13}\nabla\cdot(\nabla h)^3+\eta$ with $\nu_2<0$ and $\lambda_{13}>0$ is studied in 1+1 dimensions. Even when the value of λ_{13} is smaller than that of ν_2, the equation is shown to belong to the EW universality class. The surface current $j(m,t)$, where m is the slope of the titled surface, is also investigated and the effective ν_2 is given as $\nu_2^{\mathrm{eff}}(t)=-j'(m=0,t)\approx\nu_2+3\langle(\nabla h)^2\rangle$ for small m. Then the λ_{13} term is believed to result in a positive effective ν_2 and subsequently lead to a downhill current. The case here for the WV model is similar and the effective ν_2 can be written as $\nu_2^{\mathrm{eff}}(t)\approx\langle(\nabla h)^2[3\lambda_{13}+5\lambda_{15}(\nabla h)^2]+(\nabla h)^6[7\lambda_{17}+9\lambda_{19}(\nabla h)^2]+\cdots\rangle$. When the fluctuation caused by the instability grows rapidly with time, the positive λ_{15} nonlinearity is expected to balance the negative λ_{13} term; so is λ_{19} to λ_{17}, etc. The fluctuation saturates until a positive effective ν_2 is produced. This process is consistent with the observation of the computer simulation for the WV model [20], in which the step height fluctuation grows rapidly and saturates at a very late time.

Although the discussion above is just phenomenological and qualitative and needs to be verified by further extensive work, we can expect that the WV model governed by Eq. (2) without the $\nabla^2 h$ term is of EW type. From the terms in Eq. (2), one can expect the crossover behaviors that have been found by computer simulations [16,17]. The long time needed to observe the crossover to EW behavior may be due to the very small value of coefficients λ_{12n+1} of $\nabla\cdot(\nabla h)^{2n+1}$ nonlinearities.

III. GROWTH EQUATION FOR THE DAS SARMA–TAMBORENEA MODEL

The DT model is also a random-deposition model and the growth rule is [6] that the deposited particles can relax into the nearest kink sites. In the WV model the particles deposited at kink sites with coordination number $N_c=2$ will move to trapping sites with $N_c=3$, while they will stay at kink sites in the DT model. Moreover, in contrast to the WV model, the particles deposited at single-bond sites with $N_c=1$ choose the nearest kink or trapping sites with the same possibility. Consequently, there is no distinction between kink sites and trapping sites in the DT model.

The procedure of deriving the continuum growth equation of the DT model is similar to that of the WV model in Sec. II. The first step is to write down the transition rate according to the growth rule. The forms of $W(\mathbf{H},\mathbf{H}')$ and the transition moments $K_i^{(1)}$ and $K_{ij}^{(2)}$ are the same as those of Eqs. (11), (17) and (18), but $w_k^{(1)}$,$w_k^{(2)}$, and $w_k^{(3)}$ are different because of the different growth rule. They are written as

$$\begin{aligned} w_k^{(1)}=&\Theta(h_{k-1}-h_{k-2})\Theta(h_{k+1}-h_{k+2})\delta(h_{k-1},h_k)\\ &\times\delta(h_k,h_{k+1})+[1-\Theta(h_k-h_{k-1})]\Theta(h_k-h_{k+1})\\ &+\Theta(h_k-h_{k-1})[1-\Theta(h_k-h_{k+1})]\\ &+[1-\Theta(h_k-h_{k-1})][1-\Theta(h_k-h_{k+1})], \end{aligned} \tag{26}$$

$$\begin{aligned} w_k^{(2)}=&\delta(h_{k-1},h_k)\delta(h_k,h_{k+1})[1-\Theta(h_{k-1}-h_{k-2})]\\ &\times\left(\Theta(h_{k+1}-h_{k+2})+\frac{1}{2}[1-\Theta(h_{k+1}-h_{k+2})]\right)\\ &+\delta(h_k,h_{k+1})[1-\Theta(h_{k-1}-h_k)]\left(\Theta(h_{k+1}-h_{k+2})\right.\\ &\left.+\frac{1}{2}[1-\Theta(h_{k+1}-h_{k+2})]\right)+\frac{1}{2}\delta(h_k,h_{k-1})\\ &\times[1-\Theta(h_{k-1}-h_{k-2})][1-\Theta(h_{k+1}-h_k)]\\ &+\frac{1}{2}[1-\Theta(h_{k-1}-h_k)][1-\Theta(h_{k+1}-h_k)], \end{aligned} \tag{27}$$

$$\begin{aligned} w_k^{(3)}=&\delta(h_{k-1},h_k)\delta(h_k,h_{k+1})[1-\Theta(h_{k+1}-h_{k+2})]\\ &\times\left(\Theta(h_{k-1}-h_{k-2})+\frac{1}{2}[1-\Theta(h_{k-1}-h_{k-2})]\right)\\ &+\delta(h_{k-1},h_k)[1-\Theta(h_{k+1}-h_k)]\left(\Theta(h_{k-1}-h_{k-2})\right.\\ &\left.+\frac{1}{2}[1-\Theta(h_{k-1}-h_{k-2})]\right)+\frac{1}{2}\delta(h_k,h_{k+1}) \end{aligned}$$

$$[1-\Theta(h_{k-1}-h_k)][1-\Theta(h_{k+1}-h_{k+2})]$$

$$+\frac{1}{2}[1-\Theta(h_{k-1}-h_k)][1-\Theta(h_{k+1}-h_k)], \qquad (28)$$

and it is easy to check that they also obey the identity (16).

The next is the regularization procedure. Using the same expanding method as for the WV model and inserting (26)–(28) into (17) and (18), we have, up to $O(a^5)$,

$$K^{(1)}(x)=\frac{a}{\tau}\left[1-A_1 a^4\frac{\partial^4 h}{\partial x^4}+(-A_1^2+2A_2)a^4\frac{\partial^2}{\partial x^2}\left(\frac{\partial h}{\partial x}\right)^2\right]+O(a^6),$$

$$K^{(2)}(x,x')=\frac{a^2}{\tau}\delta(x-x')+O(a^6). \qquad (29)$$

Therefore, from Eq. (8) we obtain that the DT model is governed by the continuum growth equation (3), which is the VLD equation. The coefficients ν_4, λ_{22}, and F in Eq. (3) are the same as those in Eq. (24) and the noise η is given by the same formula (25). As discussed in Sec. II, $A_1>0$ and then $\nu_4>0$ and $\lambda_{22}<0$. According to the argument by Kim, Park, and Kim [7], we note that since in the DT model the particle landing at a single-bond site relaxes to the nearest kink site, in contrast to the case discussed by Lai and Das Sarma [10] or the conserved RSOS model [7], the surface current is generated from the lower-sloped region to the higher-sloped region. From Eq. (3) we can write the surface current as $\nabla[\nu_4\nabla^2 h-\lambda_{22}(\nabla h)^2]$; thus it can be argued roughly [7,8] that λ_{22} should be negative in the DT model, which is in agreement with our derivation.

There is no $\lambda_{13}\nabla\cdot(\nabla h)^3$ nonlinearity in above derivation for the DT model, but the EW term will be generated if the nonlinearities $\nabla\cdot(\nabla h)^{2n+1}$ exist in a higher-order expansion. If so, the surface current would appear, but previous work showed that there is no surface current in the DT model [14]. To investigate the model more explicitly, we expand $K_i^{(1)}$ to higher orders and obtain results similar to those for the WV model except for the terms $\nabla\cdot(\nabla h)^{2n+1}$, that is, as in the WV model the terms of $O(a^{2n})$ for $K_i^{(1)}$ vanish, because of the isotropic growth in the DT model, and the linear terms $\nabla^{2n+2}h$, the nonlinearities $\nabla^{2m-1}\cdot(\nabla h)^{2n+1}$ $(m\neq 1)$, and $\nabla^{2m}(\nabla h)^{2n}$ are derived. Thus the nonlinearities $\nabla\cdot(\nabla h)^{2n+1}$ do not arise and consequently no EW term is generated in the DT model. The physical origin of this result can be obtained from the microscopic process of the model, which will be discussed in Sec. IV. Therefore, in the absence of $\nabla\cdot(\nabla h)^{2n+1}$ terms, the most relevant term is $\nabla^2(\nabla h)^2$, which can be generated also from higher-order terms $\nabla^2(\nabla h)^{2n}$ [31], and we have the conclusion that the DT model obeys the scaling properties of VLD type with the exponents $\alpha=(5-d)/3$, $\beta=(5-d)/(7+d)$, and $z=(7+d)/3$.

IV. DISCUSSION AND CONCLUSION

We have obtained the continuum growth equations for the WV and DT models of the ''ideal'' MBE using the master-equation method and regularization procedure. Although the continuum equation are derived in the one-dimensional substrate growth, it is straightforward to generalize to the isotropic two-dimensional case. The growth equations derived here show that these two similar growth models belong to different universality classes. The physical process of the WV model is governed by the conserved continuum equation (2) without the EW term. But this model is expected to belong to the EW universality because of the $\nabla\cdot(\nabla h)^{2n+1}$ nonlinearities. It is interesting that we derive the VLD growth equation for the DT model. Although this result is in accordance with the recent suggestions [2,21], it does not satisfy the numerical simulations before [6,4,19].

The only difference between the derived growth equations of the WV and the DT model is the $\nabla\cdot(\nabla h)^{2n+1}$ nonlinearities. The WV model with these terms is expected to obey the EW behavior, but the DT model will not. This difference between the two continuum equations is physically attributed to the difference between the basic microscopic processes of the two growth models. In $1+1$ dimensions the WV model allows only downward jumps and generates the downhill surface current that leads to the scaling properties of the EW class. It has been pointed out by Krug, Plischke, and Siegert [14] that there is no surface current in $1+1$ dimensions if no distinction is made between kink sites and trapping sites and any net current is generated in the WV model solely on account of the events in which a particle has a choice between a trapping site and a kink site. But as shown from the growth rule in Sec. III, the particles make no distinction between trapping sites and kink sites in the DT model. Therefore, this symmetry possessed by the DT model cannot generate the surface current explicitly and subsequently cannot lead to the EW behavior, that is, it will not generate the $\nabla\cdot(\nabla h)^{2n+1}$ nonlinearity.

Since with the exception of the difference discussed above these two models obey the same growth rule, we can obtain the VLD growth equation of the DT model directly from that of the WV model by precluding the $\nabla\cdot(\nabla h)^{2n+1}$ terms, which induces the EW behavior, from Eq. (2). Moreover, from the derivations in Secs. II and III we note that in both Eqs. (2) and (3), the explicit expressions for the coefficients of $\nabla^4 h$ and $\nabla^2(\nabla h)^2$ terms are the same, and so are the forms of higher linear and nonlinear terms. This reflects the similarities between the microscopic processes of two discrete models.

From the two growth equations describing the WV and DT models, the crossover behaviors can be expected. Because of the similarities between the growth equations (2) and (3) that we have derived and also the growth rules, these two models will show similar behavior on short time and length scales, although they asymptotically belong to different universality classes and the scaling behavior of Herring-Mullins equation (1) obtained by former simulations can be considered as a transient effect. A number of numerical studies have been done to observe the crossover effects and show the EW scaling behavior for the WV model. But for the DT model, further extensive simulations need to be carried out to verify the above conclusion.

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