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Noise reduction and universality in limited-mobility models of nonequilibrium growth

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We show that a multiple-hit noise reduction technique involving the acceptance of only a fraction of the allowed atomistic deposition events could, by significantly suppressing the formation of high steps and deep grooves, greatly facilitate the identification of the universality class of limited-mobility discrete solid-on-solid conserved nonequilibrium models of epitaxial growth. In particular, the critical growth exponents of the discrete one-dimensional molecular-beam-epitaxy growth model are definitively determined using the noise reduction technique, and the universality class is established to be that of the nonlinear continuum fourth-order conserved epitaxial growth equation. [S1063-651X(98)51305-0]

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In 1991, Das Sarma and Tamborenea introduced [1] an extremely simple one-dimensional ($d=1+1$) instantaneous relaxation limited-mobility conserved discrete solid-on-solid model of ideal molecular-beam-epitaxial (MBE) growth under random vapor deposition nonequilibrium growth conditions. In spite of the deceptively simple deposition and relaxation-incorporation rules controlling its growth dynamics, the universality class of this discrete growth model, particularly in $d=1+1$ dimensions, has remained controversial [2,3] and unresolved in spite of a substantial body of work [4–11]. Our lack of understanding of the universality class of this one-dimensional growth model [1] is particularly mysterious for the following three reasons: (1) recent large scale simulations [12] of the corresponding two-dimensional ($d=2+1$) growth model seem to fairly unambiguously indicate the $2+1$ -dimensional growth universality class to be that of the fourth-order nonlinear conserved MBE growth equation [13]; (2) a number of theoretical approaches based on the kinetic master equation technique [14–16] as well as symmetry arguments [9] lead to the conclusion that the one-dimensional model should belong to the fourth-order nonlinear conserved MBE growth equation; (3) extensive large scale simulations (using up to 10^{14} deposited atoms in the largest simulations) in $d=1+1$ produce [4–9] excellent scaling of the dynamically evolving surface roughness, with

the scaling exponents, however, being approximately consistent with the *linear* fourth-order conserved growth equation [13] rather than the expected nonlinear one (with the additional complication [7,8] of there being substantial skewness in the growth morphology, implying that a *linear* description cannot apply). In addition, the model exhibits an intriguing anomalous multiscaling [6–12] behavior in the height correlation functions, which transcends the standard self-affine dynamic scaling ansatz. In this paper we obtain the elusive “correct” asymptotic universality class of this one-dimensional [1] discrete growth model by introducing a multiple-hit noise reduction scheme that has earlier been successful [17,18] in the identification of the growth universality classes for Eden and ballistic deposition models. Our noise reduction results establish that the discrete limited-mobility growth model introduced in Ref. [1] does indeed belong to the fourth-order *nonlinear* conserved MBE growth equation.

Our growth model [1] is shown in Fig. 1, where we also show the dynamical growth morphologies for the original model and the noise-reduced model. The noise reduction scheme rescales time by the noise reduction factor m (where m is the number of attempts required at a site for an actual deposition process to occur— $m=1$ in the original model of Ref. [1]), and all our times are given in terms of this rescaled time (which also defines the average film thickness in our

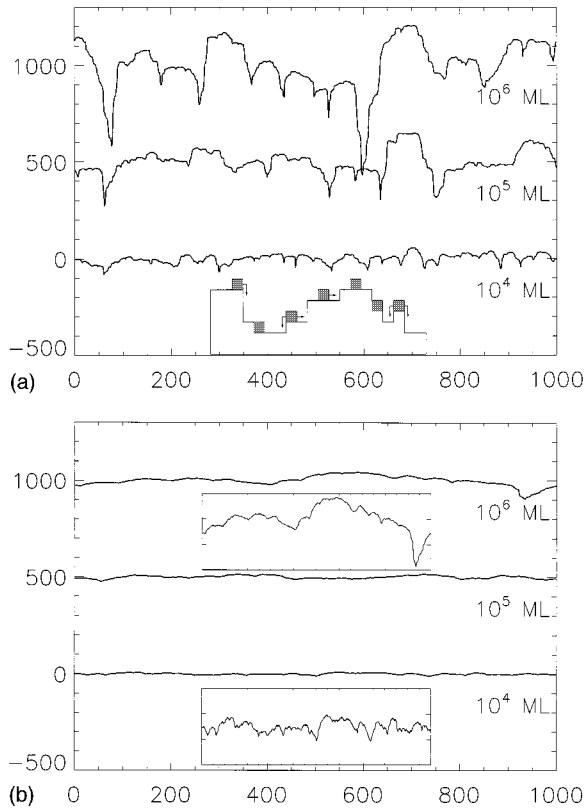


FIG. 1. (a) Dynamical morphologies from the system of substrate size $L=1000$ at 10^4 , 10^5 , and 10^6 monolayers (ML) for the original model, i.e., $m=1$. Inset: schematic configuration defining growth rules in 1+1 dimensions; m hits are needed at a site for an actual deposition event ($m=1$ in Ref. [1]). (b) Morphologies from the $m=10$ model plotted on the exact same scale as in (a), showing the much smoother surfaces. The small insets show the morphologies at 10^4 and 10^6 ML in appropriately expanded scales so that the detailed rough morphology can be seen.

model). The most striking aspect of Fig. 1 is that noise reduction is seen to have a drastic effect on the growth morphology—it strongly reduces the high surface steps and deep grooves which were the hallmark of the original [1] limited-mobility growth model. This suppression of high steps (equivalently, the reduction of local slopes) in the growing surface is, in fact, the key to the success of the noise reduction scheme in obtaining the asymptotically correct universality class of the growth model. We emphasize, however, that noise reduction, while drastically suppressing surface high steps/deep grooves, still produces a skewed growth morphology where the up-down symmetry of the starting flat substrate is spontaneously broken by the nonequilibrium growth process—in fact, the measured skewness in the growth morphology is found to be independent of the noise reduction scheme. The skewness (≈ -0.5) in the growth morphology (even in its saturated steady state) is a unique characteristic of the nonequilibrium growth model of Ref. [1] which is not shared by the other limited-mobility epitaxial growth models [19,20] existing in the literature.

To proceed further, we use the dynamical scaling ansatz, and discuss the evolving surface kinetic roughness in terms of two independent critical exponents β and α . The interface width or the root-mean-square fluctuation in the dynamical surface height $h(x,t)$, where h is the height of the growing surface at (reduced) time t at the substrate spatial point x , is

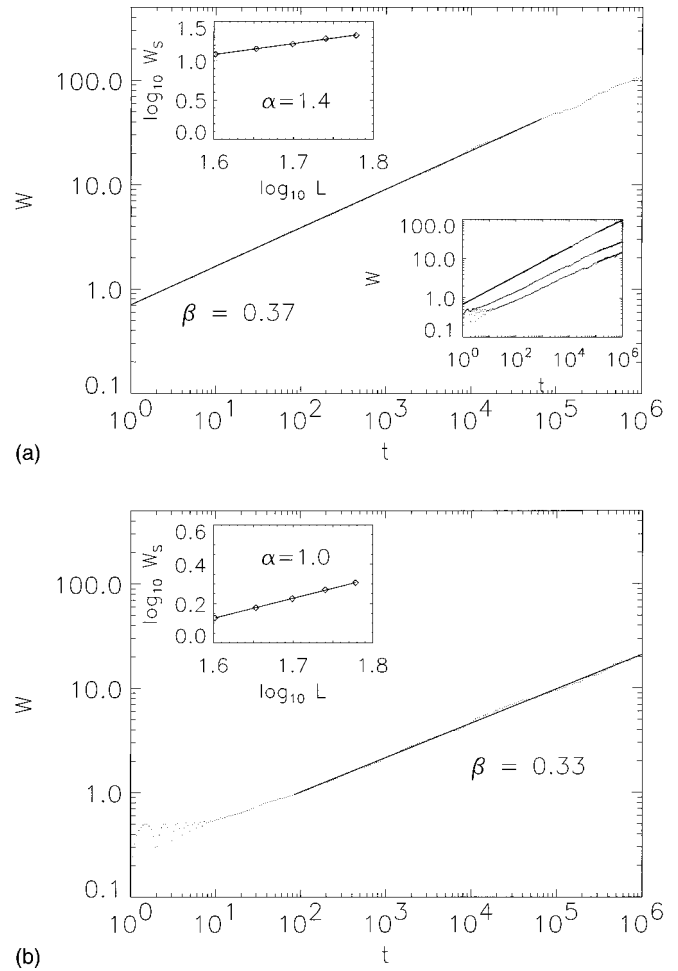


FIG. 2. Interface width $W(t)$ as a function of deposition time. Solid lines indicate the power-law fit with the growth exponent β for system $L=1000$ with (a) $m=1$ and (b) $m=10$. Inset: plots of $\log_{10}W_s$ vs $\log_{10}L$, where W_s is the saturation width. Slopes yield the roughness exponent α . Right-hand inset in (a): $W(t)$ for WV model with $m=1, 5$, and 15 from top to bottom. In the original model ($m=1$) $\beta \approx 0.36$, whereas in the noise-reduced ($m=5, 15$) results $\beta \approx 0.26$.

defined as $W(L,t) \equiv \langle (h - \langle h \rangle)^2 \rangle^{1/2}$, with the angular brackets representing the average over the substrate of width L (in the one-dimensional x direction) as well as a noise ensemble average. The dynamic scaling ansatz (which is obeyed extremely well by our results for all values of the noise reduction factor $m=1-15$ we investigated) asserts that $W(L,t) \sim t^\beta$ for $\xi \ll L$ and $W(L,t \rightarrow \infty) \equiv W_s(L) \sim L^\alpha$ in the saturated steady state for $\xi \gg L$, where the lateral correlation length $\xi \equiv \xi(t) \sim t^{1/z}$. The growth (roughness) exponent(s) $\beta(\alpha)$ and the dynamical exponent $z = \alpha/\beta$ (which describes the approach to the steady state associated with the growth of lateral correlations) completely define the universality class of the growth model, provided the growth problem is self-affine. In Fig. 2 we show our calculated $W(t)$ and $W_s(L)$ dynamic scaling plots for various values of the noise reduction factor. While all the results show excellent dynamic scaling, it is clear that the critical exponents for the noise-reduced model are $\beta \approx 0.33$, $\alpha \approx 1.0$, $z \approx 3$, whereas the original model ($m=1$) gives $\beta \approx 0.37$, $\alpha \approx 1.4$, $z \approx 3.9$, in agreement with earlier findings [1,4,7–11]. We believe that the critical exponents $\beta \approx 0.33$, $\alpha \approx 1.0$, $z \approx 3$ are the correct asymptotic exponents defining the universality class of the

one-dimensional growth model originally introduced in Ref. [1], and that the noise reduction scheme successfully suppresses the correction to scaling that dominates the $m=1$ version of the model for many decades in time.

The coarse-grained continuum equation which is believed [7–11] to describe the growth model of Ref. [1] is the conserved nonlinear MBE growth equation [13]:

$$\frac{\partial h}{\partial t} = -\nu_4 \frac{\partial^4 h}{\partial x^4} + \lambda_4 \frac{\partial^2}{\partial x^2} \left(\frac{\partial h}{\partial x} \right)^2 + \sum_{n=3}^{\infty} \lambda_{2n} \frac{\partial^2}{\partial x^2} \left(\frac{\partial h}{\partial x} \right)^{2n} + \eta, \quad (1)$$

where $h \equiv h(x, t)$ is now the height fluctuation $h - \langle h \rangle$ around the average surface height, and $\eta(x, t)$ is the (white) shot noise associated with the deposition beam fluctuations that produce the kinetic surface roughening. The critical exponents for the corresponding fourth-order *linear* equation [1,20], where $\lambda_4 = \lambda_{2n} = 0$, are trivially known to be $\beta = 0.375$, $\alpha = 1.5$, $z = 4$. It was already noted in Ref. [1] that the simulated growth exponents of the discrete model seem to be following those of the linear version of Eq. (1) although no particular significance was attached to this fact. The intriguing aspect of the critical behavior of the discrete model in $d=1+1$ dimensions has been its consistency with the linear version of Eq. (1) as far as the *global* exponents β (≈ 0.375), α (≈ 1.5), and z (≈ 4) go, whereas at the same time the up-down symmetry of the growth problem, which is manifestly present in the linear equation because $h \rightarrow -h$ leaves the equation invariant, is broken with the evolving growth morphology, explicitly showing a finite skewness $s = \langle h^3 \rangle \langle h^2 \rangle^{-3/2} \approx -0.5$ (obviously $s \equiv 0$ for the linear equation). Thus the puzzle until our current work has been that the one-dimensional discrete growth model should *not* belong to the fourth-order conserved linear growth equation universality, except that it does for as long as (at least up to eight decades in time) one can dynamically simulate the model [1–12]. Our multiple-hit noise reduction scheme resolves the mystery by obtaining the asymptotic exponents by successfully eliminating the problem of severe correction to scaling, which hinders the $m=1$ version [1] of the model. This is similar to what was earlier found in the Eden model [17,18].

The critical exponents we obtain in the noise-reduced model ($\beta \approx 0.33$, $\alpha \approx 1.0$, $z \approx 3$) are consistent with the one-loop dynamical RG [13] treatment ($\beta = 1/3$, $\alpha = 1$, $z = 3$) and direct numerical simulations [11,21] of the *fourth-order nonlinear conserved MBE* growth equation [13] with $\lambda_{2n} = 0$, but $\nu_4, \lambda_4 \neq 0$ in Eq. (1). The original thinking [13], that these one-loop results may in fact be exact for the fourth-order nonlinear equation, has recently been questioned [22] with a two-loop dynamical renormalization group (RG) treatment obtaining miniscule (less than 0.5%) numerical corrections. These two-loop corrections are too small to be of any practical significance in our work (or to other simulations and experiments). We therefore conclude that the critical exponents of the noise-reduced version of the growth model introduced in Ref. [1] are the same as those of Eq. (1) with $\lambda_{2n} \equiv 0$ for $n \geq 3$, and therefore the model belongs to the universality class of the nonlinear fourth-order conserved MBE growth equation.

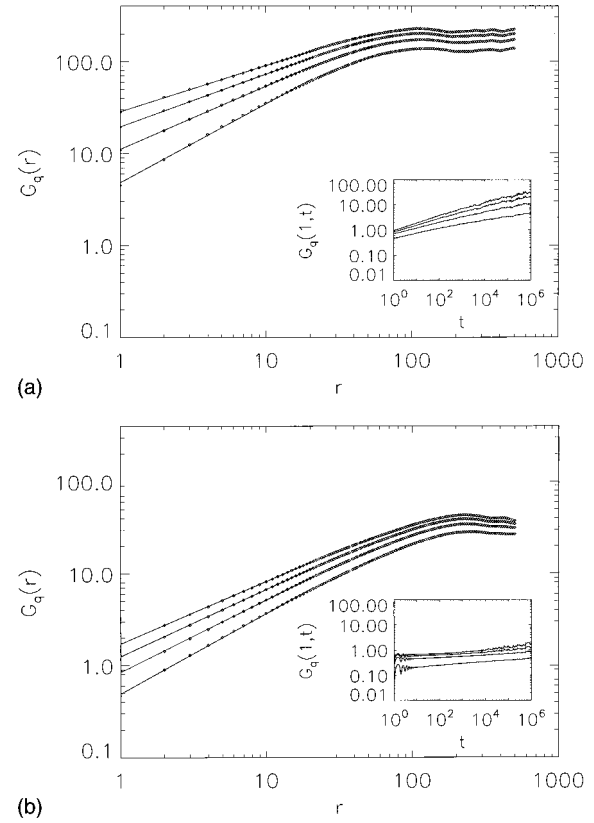


FIG. 3. (a) Anomalous multiscaling behavior of the height correlation functions $G_q(r, t) = \langle |h(x+r, t) - h(x, t)|^q \rangle^{1/q}$ at fixed $t = 10^6$ ML and the nearest-neighbor height difference correlation functions $G_q(1, t) = \langle |h(x+1, t) - h(x, t)|^q \rangle^{1/q}$ (inset) with $q = 1-4$ from bottom to top. Substrate size $L = 1000$ and $m = 1$. (b) The same plots for the system with $m = 10$. The noise-reduced correlation functions show only very weak anomalous multiscaling behavior.

We believe that the success of noise reduction in producing the correct asymptotic growth universality arises from the suppression of the infinite series of nonlinear term ($\lambda_{2n} \neq 0$) in Eq. (1) which are associated with the high steps in the original ($m=1$) discrete growth model [1]. The role of the infinite series of nonlinear terms (i.e., $\lambda_{2n} \neq 0$ for $n = 3, 4, \dots$) in Eq. (1) is quite subtle [10,11] because the existence of such an infinite series of *relevant* terms is unusual in critical phenomena. High steps, however, imply large values of the slope $\partial h / \partial x$, indicating the existence of the infinite series. Simple power counting shows all the terms in this infinite series to be *marginally relevant operators* in the one-dimensional growth problem, and since they are all allowed by the symmetry of the discrete model, they should all be present [7,11] in the growth model of Ref. [1]. Note that the corresponding linear problem has $\alpha (= 1.5) > 1$, implying that the infinite nonlinear series should be generated if allowed by symmetry. This infinite series has recently been shown [10,11] to be responsible for giving rise to the anomalous “intermittent” multiscaling behavior in the growth model of Ref. [1], which has attracted considerable attention [6–11]. In Fig. 3 we show that the noise reduction technique essentially eliminates the anomalous multiscaling behavior in the height correlation functions of the growth model of Ref. [1]. Thus the noise reduction technique resolves all three of the intriguing and puzzling features of the one-dimensional minimal MBE growth model of Ref. [1],

namely, (1) it establishes beyond any reasonable doubt the correct universality class of the model to be the “expected” fourth-order conserved nonlinear continuum growth equation; (2) it suppresses the “unphysical” feature of high steps and deep grooves in the growth morphology while maintaining a finite skewness in the morphology; (3) it suppresses the anomalous multiscaling in the model.

Before concluding, we emphasize an important feature of our growth model characterized by what is *absent* from Eq. (1)—the well-known [9,23,24] Laplacian $\nu_2(\partial^2 h)/(\partial x^2)$ term associated with the generic Edwards-Wilkinson (EW) universality class is strictly absent from the growth equation describing the discrete growth model of Ref. [1]. The model of Ref. [1] is, in fact, the only known limited-mobility MBE growth model *that does not belong to the generic EW growth universality class*. It is worth emphasizing this point because this has been a controversial and contentious [2,3,9,25] issue in the past.

To reinforce this point we have also carried out noise reduction simulations of the closely related Wolf-Villain (WV) model [20], which differs from the model of Ref. [1] only in that all deposited atoms, *independent of their initial coordinations*, are allowed to move to lateral nearest-neighbor sites in order to *maximize* their local coordination number. Although it is well-accepted [9,25] that the WV model asymptotically belongs to the EW universality class, this crossover has never been clearly observed in simulations because for all practical purposes the dynamic scaling behavior of the WV model [20] is similar to that of the model of Ref. [1] up to the longest simulation times. Our $d=1+1$ noise-reduced WV model simulations, shown as an inset in Fig. 2(a), clearly show that the asymptotic growth exponent β decreases from ~ 0.36 (for $m=1$) to $\sim 0.26 = \beta_{EW}$ in $d=1+1$ (for $m=15$) under the noise reduction technique. Thus the WV model belongs to the EW universality and the model of Ref. [1] belongs to the fourth-order nonlinear MBE growth universality.

The nonexistence of the EW term [which, if it existed, would have defined the universality class of the model because all of the fourth-order terms in Eq. (1) are *irrelevant* compared with the EW Laplacian term] in the growth model of Ref. [1] is, in fact, an exact result due to a hidden sym-

metry [9] in the growth model that produces an exactly vanishing surface current [25] in the model on a tilted substrate. The surface current on a tilted substrate is, in general, proportional [9,25] to the strength ν_2 of the generic EW term in the growth equation, and therefore its vanishing implies $\nu_2 \equiv 0$. Our calculated inclination-dependent surface current on a tilted substrate in the growth model is essentially zero within error bars for all values of the noise reduction factor ($m=1-15$). This is also a strong indication that noise reduction does not change the universality class of our growth model. This is similar to what was found earlier [17,18] in the Eden model. It may be worthwhile to point out that in the Eden model also [17,18] the success of noise reduction in eliminating corrections to scaling arises from the suppression of high steps.

We conclude by discussing why understanding the universality class of the growth model introduced in Ref. [1] is of considerable interest. An important theoretical reason is that this model is the *only* limited-mobility MBE growth model that does not belong to the generic EW universality class and therefore, as an exception, its proper theoretical understanding is of obvious interest. The fact that this growth model exhibits complex and highly nontrivial anomalous multifractal dynamic scaling [6–11] is an additional theoretical incentive in understanding its growth universality. Another significant feature is that, by construction, this growth model is the low-temperature version [1,4] of the full temperature-dependent activated diffusion MBE growth model [4,8] because in the limited-mobility model only the adatoms without any lateral bonding are allowed to increase their coordination through diffusion and therefore it has considerable experimental significance. It may be appropriate in this context to point out that several experimental measurements [26] of MBE growth exponents ($\beta \approx 0.2$, $\alpha \approx 0.7$) are consistent with the ($d=2+1$ dimensional) critical exponents given by the fourth-order nonlinear conserved growth equation which, as we show in this paper and in Ref. [12], defines the universality class of the limited-mobility discrete growth model of Ref. [1].

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