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Numerical evidence for anomalous dynamic scaling in conserved surface growth

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ABSTRACT

According to the scaling idea of local slope, we investigate the anomalous dynamic scaling of a class of nonequilibrium conserved growth equations in (1+1)- and (2+1)-dimensions using numerical integration. The conserved growth models include the linear Molecular-Beam Epitaxy (LMBE), the nonlinear Villain–Lai–Das Sarma (VLDS) and Sun–Guo–Grant (SGG) equations. To suppress the instability in the VLDS and SGG equations, the nonlinear terms are replaced by exponentially decreasing functions. The critical exponents in different growth regions are obtained. Our results are consistent with the corresponding analytical predictions. The anomalous scaling properties are proved in (1+1)-dimensional LMBE and VLDS equations for Molecular-Beam Epitaxy (MBE) growth. However, anomalous roughening in the LMBE and VLDS surfaces is very weak in the physically relevant case of (2+1)-dimensions. Furthermore, we find that, in both (1+1)- and (2+1)-dimensions, anomalous scaling behavior does not appear in the SGG surface based on scaling approach and numerical evidence.

1. Introduction

The study of growing interfaces has been a very active field for many years. Many studies focus on the technologically relevant growth of thin films or nanostructures, and growing interfaces are also encountered in various other physical, chemical, or biological systems, ranging from bacterial growth to diffusion fronts. Over the years important insights into the behavior of non-equilibrium growth processes have been gained through the study of simple model systems that capture the most important aspects of real experimental systems [1–4].

In the dynamic scaling theory of surface roughening, one of the successful approaches to study the scaling behavior of growing surfaces is by formulating continuum Langevin-type equations which are assumed to incorporate the physics of growth processes and then applying analytical or numerical analysis to the growth equations so as to determine their scaling properties. The conserved growth equations with additive noise are generally used to model nonequilibrium surface growth in Molecular-Beam Epitaxy (MBE). The conservation is a consequence of absence of bulk vacancies, overhangs, and desorption (evaporation of atoms from the substrate) under optimum MBE growth conditions. Thus, integrating over the whole sample area gives the number of particles deposited.

In a coarse-grained picture, the growing surface is described by the height $h(\vec{r},t)$, which is a continuous function of spatial variable $\vec{r}$ and growth time t. Generally, one can describe stochastic (Langevin) differential equations for surface evolution in the form

$$\frac{\partial h\left(\vec{r},t\right)}{\partial t} = \Re\left\{\nabla h\left(\vec{r},t\right)\right\} + \xi_{(c)}\left(\vec{r},t\right), \tag{1}$$

where $\Re(\nabla h)$ is a function of $h\left(\vec{r},t\right)$ measured in a comoving frame of reference. Surface growth is driven by external noises $\xi_{(c)}\left(\vec{r},t\right)$, which represent the influx of particles in deposition processes. The noises are usually considered to be Gaussian, zero mean, uncorrelated in space and time, and either nonconserved,

$$\left\langle \xi\left(\vec{r},t\right)\xi\left(\vec{r}',t'\right)\right\rangle = 2D\delta^d\left(\vec{r}-\vec{r}'\right)\cdot\delta\left(t-t'\right), \tag{2}$$

or conserved,

$$\left\langle \xi_c\left(\vec{r},t\right)\xi_c\left(\vec{r}',t'\right)\right\rangle = -2D_c\nabla^2\delta^d\left(\vec{r}-\vec{r}'\right)\cdot\delta\left(t-t'\right), \tag{3}$$

where d is the substrate dimension and D (or D_c) denotes the noise amplitude.

To describe MBE growth processes, one assumes that the dominant physical mechanism of surface smoothing is surface diffusion, without desorption, overhangs and bulk vacancies. These assumptions are well satisfied in a typical experimental situation for MBE growth at sufficiently high temperatures. Then the model is volume conserving and the function $\Re\{\nabla h(\vec{r},t)\}$ has a form $\Re\{\nabla h(\vec{r},t)\} = \nabla\cdot\vec{j}$, where the current $\vec{j}(\vec{r},t)$ is a function of the derivatives of $h(\vec{r},t)$. A simple possibility is $\vec{j}\propto\nabla\nabla^2 h$, which describes surface diffusion in equilibrium. The current is proportional to the gradient of chemical potential, which is, in

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turn, given by the surface curvature $\nabla^2 h$. We will refer to Eq. (1), containing only this fourth-order term, as the linear diffusion model. We call the most simple conserved growth model as linear Molecular-Beam Epitaxy (LMBE) equation [1].

In general, the current contains additional nonlinear and higher-order terms. However, asymptotically, only some of these terms may be relevant and lead to certain well-defined values of exponents. Crossover to these *true* exponents caused by asymptotically irrelevant terms may be, however, rather slow. In the context of kinetic roughening in models for MBE growth, one of the most possible nonlinear leading terms has been well studied: $\vec{j} \propto \nabla(\nabla h)^2$, the corresponding term $\nabla^2(\nabla h)^2$ in the Langevin-type equation is called the nonlinear term of a conserved growth. Then the function $\Re\{\nabla h(\vec{r},t)\}$ has a more general form $\Re = -K\nabla^4 h(\vec{r},t) + \lambda\nabla^2(\nabla h)^2$. Adding the random noise $\xi_{(c)}(\vec{r},t)$ to $\Re$, the stochastic growth equations are called Villain–Lai–Das Sarma (VLDS) equation with a nonconserved noise and Sun–Guo–Grant (SGG) equation with a conserved noise, respectively [5–7].

Although the dynamic scaling behavior of the conserved growth equations describing MBE has been extensively investigated numerically and analytically, many open problems still remain, such as anomalous scaling behavior, mound formation, and close correspondence of the continuum growth equations and the related atomistic models. The purpose of this work is to examine, in detail, kinetic roughening, anomalous scaling and critical behavior of the continuum stochastic equations for epitaxial growth processes. We study spatially discretized versions of LMBE, VLDS and SGG equations using numerical integration. The replacement of nonlinear terms in VLDS and SGG equations is used by exponentially decreasing functions to suppress instabilities. The critical exponents in different growth regions are obtained through interface width and equal-time height difference correlation function. Our numerical results concern the evidences of anomalous scaling of $(1+1)$-dimensional growth surface, which are in excellent agreement with the simple theoretical analysis: a power-counting analysis (LMBE) and Flory-type arguments (VLDS). However, our results also imply that anomalous roughening in the LMBE and VLDS surfaces is very weak in the physically relevant case of $(2+1)$-dimensions. Furthermore, we find that, whether in $(1+1)$- or $(2+1)$-dimensions, the SGG surface always exhibits normal self-affine fractal structure.

The rest of this paper is organized as follows. Section 2 contains a brief review of scaling properties in surface growth. In Section 3, the conserved growth equations and their corresponding local slopes are described, and the anomalous scaling behavior of these conserved equations is discussed according to the scaling idea of local slope. Section 4 contains the finite-difference approximations of the conserved growth equations. The exponentially decreasing functions are adopted to suppress growth instabilities in the discretized VLDS and SGG equations. In Section 5, extensive numerical results of the conserved growth equations and their local derivatives are obtained. Surface morphologies and anomalous scaling in these growth models are also discussed. The following conclusions are drawn from the present study in Section 6.

2. Scaling properties in growth surface

Growth processes have been shown to exhibit scaling properties that allow one to divide the models into universality classes [1–4]. A rough surface may be characterized by the fluctuations of the growth height around its mean value. One of the most important physical quantities related to the surface roughening is the global interface width $W(L,t)$ defined as

$$W(L,t) = \frac{1}{\sqrt{L}}\left\langle \sum_{\vec{r}}\left[h\left(\vec{r},t\right) - \overline{h}_L(t)\right]^2\right\rangle^{1/2}, \tag{4}$$

where $\overline{h}_L = (1/L)\sum_{\vec{r}} h\left(\vec{r},t\right)$ denotes the spatial average, and the brackets $\langle\cdots\rangle$ denote an average over different realizations. In many cases, starting from an initially flat surface, the global width is observed to satisfy the dynamic scaling form of Family-Vicsek [8]

$$W(L,t) = L^{\alpha} f\left(t/L^z\right), \tag{5}$$

where the scaling function $f(u)$ behaves as

$$f(u) \sim \begin{cases} u^{\alpha} & \text{if } u \ll 1, \\ const. & \text{if } u \gg 1. \end{cases} \tag{6}$$

A typical plot of the time evolution of the global width has two regions separated by a crossover time $t_\times$ ($t_\times \sim L^z$). Initially, the interface width increases as a power of time, $W(L,t) \sim t^{\beta}$ ($t \ll t_\times$), where β is called growth exponent and describes the short-time behavior of the surface. However, the power law increasing in width does not continue indefinitely, but is followed by a saturation region during which the width reaches a saturation value, $W(L,t) \sim L^{\alpha}$ ($t \gg t_\times$), where α, is called the roughness exponent, and is a second critical exponent that characterizes the roughness of the saturated interface. The ratio $z=\alpha/\beta$ is a dynamic exponent, which describes the dependence of the crossover time $t_\times$ with the system size through the relation $t_\times \sim L^z$. Two of them can determine the universality class of the growth models under study.

In addition to the global interface width, the equal-time height difference correlation function $G(l,t)$ is also very important and informative. Here, $G(l,t)$ is defined as

$$G(l,t) = \left\langle \left(h\left(\vec{r}+\vec{l},t\right) - h\left(\vec{r},t\right)\right)^2\right\rangle, \tag{7}$$

where the brackets $\langle\cdots\rangle$ denote ensemble average. The local roughness exponent α_{loc} can be determined from the relation

$$G(l,t) \sim l^{2\alpha_{loc}} \quad (l \ll L). \tag{8}$$

The relation $\alpha=\alpha_{loc}$ is always satisfied in a normal self-affine interface.

Recently, a most intriguing feature of some growth models is that the above standard Family-Vicsek scaling of the global interface width differs substantially from the scaling behavior of the local interface fluctuations (measured either by the local width or the height difference correlation function), i.e. anomalous roughening [9–15]. This leads to the existence of an independent critical exponent (i.e. α_{loc}) which characterizes the local interface fluctuations on scales $l \ll L$ and differs from the global roughness exponent α. The anomalous scaling behavior has also been widely observed experimentally, ranging from MBE growth [16,17], interface advance in porous media [18,19], material fracture surfaces [20–23], sputter-deposition growth [24–26], electrodeposition growth [27–29], even to plant callus and tumor growth [30–32].

In order to investigate anomalous dynamic behavior in growth surfaces, López et al. [10–13] proposed a new scaling function instead of the normal Family-Vicsek scaling when an anomalous roughening takes place for growth processes, and scales as

$$w(l,t) \sim t^{\beta} f_A\left(l/t^{1/z}\right), \tag{9}$$

with an anomalous scaling function given

$$f_A(u) \sim \begin{cases} u^{\alpha_{loc}} & \text{if } u \ll 1, \\ const. & \text{if } u \gg 1, \end{cases} \tag{10}$$

instead of Eq. (5). The normal self-affine Family-Vicsek scaling [8] is then recovered when $\alpha=\alpha_{loc}$.

It is important to note that the mean square local slope (average surface gradient) has a nontrivial dynamics [10–13]. The local slope