Evidence for the anomalous scaling behaviour of the molecular-beam epitaxy growth equation*

Tang Gang(唐 刚)†, Xia Hui(夏 辉)‡, Hao Da-Peng(郝大鹏), Xun Zhi-Peng(寻之朋), Wen Rong-Ji(温荣吉), and Chen Yu-Ling(陈玉岭)

Department of Physics, China University of Mining and Technology, Xuzhou 221116, *China*

(Received 14 May 2010; revised manuscript received 10 October 2010)

According to the scaling idea of local slope, we investigate numerically and analytically anomalous dynamic scaling behaviour of $(1+1)$-dimensional growth equation for molecular-beam epitaxy. The growth model includes the linear molecular-beam epitaxy (LMBE) and the nonlinear Lai–Das Sarma–Villain (LDV) equations. The anomalous scaling exponents in both the LMBE and the LDV equations are obtained, respectively. Numerical results are consistent with the corresponding analytical predictions.

Keywords: molecular-beam epitaxy, surface growth equation, anomalous scaling behaviour

PACS: 64.60.Ht, 05.40.–d, 05.70.Ln **DOI:** 10.1088/1674-1056/20/3/036402

1. Introduction

The growing interfaces have been studied as 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 behaviour 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 studying the scaling 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.[1−3] Generally, the Langevin-type equation can be described as

$$\frac{\partial h(x,t)}{\partial t} = \Re(\nabla h) + \eta(x,t), \tag{1}$$

where $h(x,t)$ is the height of the interface at substrate position. The function $\Re(\nabla h)$ defines a particular model and incorporates the relevant symmetries and conservation laws. Surface growth is driven by an external noise $\eta(x,t)$, which represents the influx of particles in deposition processes. The noise is usually considered to be Gaussian, zero mean and uncorrelated in space and time

$$\langle \eta(x,t)\eta(x',t')\rangle = 2D\delta(x-x')\cdot\delta(t-t'), \tag{2}$$

where D denotes the noise amplitude.

Growth processes have been shown to exhibit scaling properties that allow one to divide the models into universality classes.[1−3] A rough surface may be characterized by the fluctuation of the growth height around its mean value, the basic quantity concerned is the global interface width $W(L,t)$, which satisfies the scaling form, and is scaled according to the Family–Vicsek ansatz[5] as

$$W(L,t) = L^{\alpha} f(t/L^{z}), \tag{3}$$

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

$$f(u) \sim \begin{cases} u^{\alpha}, & \text{if} \quad u \ll 1, \\ \text{const}, & \text{if} \quad u \gg 1. \end{cases} \tag{4}$$

The roughness exponent α and the dynamic exponent z describe the asymptotic behaviours of the growing interface on the large length scale and the long-time scale, and determine the universality class of the model under study. The ratio $\beta = \alpha/z$ is called growth exponent and characterizes the short-time behaviour of the surface.

*Project supported by the Fundamental Research Funds for the Central Universities (Grant No. 2010LKWL04), and the Youth Foundation of China University of Mining & Technology, China (Grant No. 2008A035).

†Corresponding author. E-mail: gangtang@cumt.edu.cn

‡Corresponding author. E-mail: xiahui_cumt@163.com

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The scaling picture above has been successfully applied to a great variety of growth models, which include, for instance, the important universality classes associated with the Edwards–Wilkinson (EW)[6]and Kardar–Parisi–Zhang (KPZ)[7] equations. However, 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 behaviour of the local interface fluctuations (measured either by the local width or by the height–height correlation function), i.e., anomalous roughening.[8−14] This leads to the existence of an independent local roughness exponent $\alpha_{\rm loc}$ which characterizes the local interface fluctuations on scales $l \ll L$ and differs from the global roughness exponent α.

For the sake of arguing the interesting question, we investigate the anomalous scaling properties of the stochastic equations describing molecular-beam epitaxy (MBE) growth, including the linear molecular-beam epitaxy (LMBE) and the nonlinear Lai–Das Sarma–Villain (LDV) equations. We show that local derivatives of the Langevin-type equations describing MBE growth lead to new phases. We find numerical support for the existence of anomalous scaling behaviour in the MBE growth system in $(1+1)$-dimensions. Our numerical results concern the evidences of anomalous scaling of surface, and are in excellent agreement with the simple theoretical analysis: a power-counting analysis (LMBE) and Flory-type arguments (LDV).

The rest of this paper is organized as follows. In Section 2 we give a brief review of scaling of local slopes in surface growth. In Section 3, we describe MBE equations and the corresponding local derivatives, and discuss the anomalous scaling behaviour of the equations. Power-counting analysis and a Flory-type approach are used to obtain anomalous scaling exponents, separately. In Section 4 we show the finite-difference approximations and numerical results of the local derivatives of MBE equations in (1+1)-dimensions. The conclusions are drawn from the present study in Section 5, finally.

2. Scaling of local slope in surface growth

In order to investigate anomalous dynamic behaviour in growth surfaces, López *et al.*[10−13] proposed a new scaling function to replace the normal Family–Vicsek scaling when an anomalous roughening takes place for growth processes, and scaled it as

$$w(l,t) \sim t^{\beta} f_A(l/t^{1/z}), \tag{5}$$

with an anomalous scaling function given as

$$f_A(u) \sim \begin{cases} u^{\alpha_{\rm loc}}, & \text{if} \quad u \ll 1, \\ \text{const}, & \text{if} \quad u \gg 1 \end{cases} \tag{6}$$

replacing Eq. (4). The normal self–affine Family–Vicsek scaling[5] is then recovered when $\alpha = \alpha_{\rm loc}$.

It is important to note that the mean square local slope (average surface gradient) has a nontrivial dynamic behaviour.[10−13] The local slope fluctuation is scaled as $\langle \overline{(\nabla h)^2} \rangle \sim t^{2\kappa}$, when $\kappa > 0$, the local slope fluctuation becomes relevant scale (in the growth direction) and local scaling behaviour is expected to be anomalous, Eq. (5), instead of the standard self–affine Family–Vicsek (3). By applying the operator ∇ to both sides of Eq. (1), the Langevin-type equation for the local derivative $\Upsilon(x,t) = \nabla h(x,t)$ reads

$$\frac{\partial \Upsilon(x,t)}{\partial t} = \nabla \Re(\Upsilon) + \nabla \eta(x,t). \tag{7}$$

Assuming periodic boundary conditions in Eq. (1) implies $\overline{\nabla h} = 0$ and one then finds that the global width of the interface $\Upsilon(x,t)$ is

$$W_{\Upsilon}(t) = \langle \overline{\Upsilon(x,t)^2 - \overline{\Upsilon(x,t)}^2} \rangle^{1/2} = \langle \overline{\nabla h^2} \rangle^{1/2}, \tag{8}$$

which immediately leads to $W_{\Upsilon}(t) \sim t^{\kappa}$.[11,13] Therefore, by studying the scaling behaviour of the surface $\Upsilon(x,t)$, one can obtain the anomalous time growth exponent κ.

López *et al.*[13] considered the slope $\Upsilon(x,t)$ as a growing surface of its own and study its roughening properties. Specifically, the time scale invariance of Eq. (8) implies that the global width is expected to obey Eqs. (3) and (4), so that the global width increases as a power of time $W_{\Upsilon}(L,t) \sim t^{\kappa}$ for the early-time regime, and saturates, $W_{\Upsilon}(L,t) \sim L^{\hat{\alpha}}$ for the long time regime, where $\hat{\alpha}$ and $\hat{z} = \hat{\alpha}/\kappa$ are the roughness and dynamic exponents of the interface defined by the local slopes, respectively. The Langevin-type growth equation, i.e. Eq. (7), may yield a surface $\Upsilon(x,t)$ that is not rough, i.e., $\hat{\alpha} < 0$ (or $\kappa < 0$). However, when $\hat{\alpha} > 0$, the corresponding local slope $\Upsilon(x,t)$ may turn rough, which straightforwardly implies anomalous scaling behaviour of the growth surface $h(x,t)$.

3. Local derivative of MBE equation

3.1. LMBE equation

The LMBE equation is expressed as [1−3]

$$\frac{\partial h(x,t)}{\partial t} = -\nu\nabla^4 h + \eta(x,t). \tag{9}$$

The first term on the right-hand side of Eq. (9) is the diffusion term, and $\eta(x,t)$ is the Gaussian white noise described by Eq. (2).

Despite its simplicity, the equation plays an important role in the theory of MBE growth. The critical exponents are easily calculated in any dimension, in particular, one has $\alpha = 3/2$ and $\beta = 3/8$ in $(1+1)$-dimensions. The model exhibits superrough interfaces ($\alpha > 1$), therefore, this leads to anomalous scaling.

By applying the operator ∇ to both sides of Eq. (9), the LMBE equation for the local derivative $\Upsilon = \nabla h$ reads

$$\frac{\partial \Upsilon(x,t)}{\partial t} = -\nu\nabla^4\Upsilon(x,t) + \nabla\eta(x,t). \tag{10}$$

The scaling exponents for Eq. (10) can be developed by a power-counting analysis as follows. The conservative noise $\nabla\eta$ is qualitatively different from the Gaussian white noise η, and satisfies $\langle\nabla\eta(x,t)\rangle = 0$ and $\langle\nabla\eta(x,t)\nabla\eta(x',t')\rangle = -2D_{\rm c}\nabla^2\delta(x-x')\cdot\delta(t-t')$.

We consider $\Upsilon(x,t)$ as a new growing interface, then on rescaling it both horizontally $x \to bx$, and vertically $\Upsilon \to b^{\hat{\alpha}}\Upsilon$. Since the interface roughness depends on time as well, to compare two interfaces obtained at different moments we must rescale the time as $t \to b^{\hat{z}}t$, and the conservative noise $\nabla\eta(x,t) \to b^{-(d+\hat{z}+2)/2}\nabla\eta(x,t)$. Then Eq. (10) can be rescaled as

$$b^{\hat{\alpha}-\hat{z}}\frac{\partial\Upsilon}{\partial t} = -\nu b^{\hat{\alpha}-4}\nabla^4\Upsilon + b^{-(d+\hat{z}+2)/2}\nabla\eta. \tag{11}$$

Multiplying both sides of Eq. (11) with $b^{\hat{z}-\hat{\alpha}}$, we obtain

$$\frac{\partial\Upsilon}{\partial t} = -\nu b^{\hat{z}-4}\nabla^4\Upsilon + b^{-(d-\hat{z}+2\hat{\alpha})/2}\nabla\eta. \tag{12}$$

To insure scaling invariance, one would expect that the terms on the right-hand side of Eq. (9) must be independent of b. The scaling exponents can be obtained as $\hat{\alpha} = (2-d)/2$ and $\hat{z} = 4$. Therefore the anomalous growth exponent $\kappa = \hat{\alpha}/\hat{z} = (2-d)/8$, which is consistent with the results obtained by a Flory approach.[15] Therefore, the width of the local interface derivative is estimated as $W_\Upsilon(L,t) \sim t^{(2-d)/8}$ in the d-dimensional substrate. It is obvious that when $d < 2$, the anomalous growth exponent κ is positive, therefore the LMBE model is expected to appear to be anomalously roughening. In the case of $(1+1)$-dimensional LMBE, the exponent $\kappa = 1/8$ illuminates the model displaying anomalous scaling.[11]

3.2. LDV equation

The nonlinear LDV equation is proposed by Lai and Das Sarma[16] and Villain[17] for describing MBE growth as follows:

$$\frac{\partial h(x,t)}{\partial t} = -\nu\nabla^4 h + \frac{\lambda}{2}\nabla^2(\nabla h)^2 + \eta(x,t). \tag{13}$$

The first term on the right-hand side is the diffusion term, the second term is nonlinear term for describing the lateral growth, and $\eta(x,t)$ is the Gaussian white noise, both ν and λ are constants.

This equation is expected to describe the behaviour of the long-wavelength fluctuations of the interface height in several discrete models of MBE growth. According to the dynamic renormalization-group analysis, the scaling exponents $\alpha = (4-d)/3$ and $z = (8+d)/3$ are expected.[16,17] However, numerical simulations of the LDV equation and several discrete growth models in the same universality class have shown that the model exhibits anomalous scaling with a local roughness exponent $\alpha_{\rm loc} < 1$ in $(1+1)$-dimensions.[8,9,11]

Correspondingly, the local derivative of the LDV equation is

$$\frac{\partial\Upsilon(x,t)}{\partial t} = -\nu\nabla^4\Upsilon(x,t) + \frac{\lambda}{2}\nabla^3\Upsilon^2(x,t) + \nabla\eta(x,t). \tag{14}$$

In the spirit of the Flory approach,[11,18] at long time $t \gg t_l$ (characteristic time $t_l \sim l^z$), and averaged over length scale l, the typical magnitude of the fluctuation in $\Upsilon(\vec{r},t)$ is scaled as Υ_l, and that these fluctuation lasts for the time on the order of t_l. The various terms in Eq. (14) may be estimated as $\langle|\partial\Upsilon/\partial t|\rangle_l \sim \Upsilon_l/t_l$, $\nu\langle|\nabla^4\Upsilon|\rangle_l \sim \nu\Upsilon_l/l^4$, $\lambda\langle|\nabla^3(\Upsilon^2)|\rangle_l \sim \lambda\Upsilon_l^2/l^3$. As for the noise term expressed in Eq. (14), one can estimate its fluctuation on length scale l and time is scaled as $\langle|\nabla\eta|\rangle_{l,\rm sc} \sim (D\Upsilon_l l^{d+1}t_l)^{-1/2}$ for rough interface.

At sufficiently large length scale, the nonlinear term dominates the curvature diffusion term, then the noise fluctuation estimated for rough interface approximately equals the inertial term, i.e., $\langle|\partial\Upsilon/\partial t|\rangle_l \sim \langle|\nabla\eta|\rangle_l$, or further $\Upsilon_l/t \sim (D\Upsilon_l l^{d+1}t_l)^{-1/2}$. thus

one can obtain $\Upsilon_l \sim \left(Dt_l/l^{d+1}\right)^{1/3}$. Equating the inertial term $\langle|\partial\Upsilon/\partial t|\rangle_l$ to the nonlinear term, i.e., $\Upsilon_l/t_l \sim \lambda\Upsilon_l^2/l^3$, we have $\Upsilon_l \sim (1/\lambda)\, l^3/t_l$. Thus, we can estimate a fluctuation of Υ_l scaled in time and length as $\Upsilon_l \sim \left(D^3/\lambda^{d+9}\right)^{1/(d+10)} t_l^{(2-d)/(d+10)}$ and $\Upsilon_l \sim (D/\lambda)^{1/4}\, l^{(2-d)/4}$, respectively.

According to the analytic results above, we obtain the scaling exponents $\kappa = (2-d)/(d+10)$, and $\hat{\alpha} = (2-d)/4$. It is obvious that when $d < 2$, the anomalous growth exponent κ is positive, therefore the LDV equation is expected to display anomalous roughening. When $d = 1$, then $\kappa = 1/11$, which illuminates the LDV equation in $(1+1)$-dimensions is expected to display anomalous roughening.

4. Numerical simulations and results

In this section, we perform numerical simulations of LMBE and LDV equations in order to check their anomalous results. From the scaling calculation results above, obtained from either LMBE or LDV equations, the anomalous behaviour appears only when $d < 2$. Thus $(1+1)$-dimensional MBE equations are the most interesting for investigating anomalous scaling behaviour.

For $(1+1)$-dimensional local derivative of LMBE model, the discrete form of Eq. (10) can be written as

$$\Upsilon(x,t+\Delta t) - \Upsilon(x,t) = -\frac{\nu\Delta t}{(\Delta x)^4}[\Upsilon(x+2\Delta x,t) - 4\Upsilon(x+\Delta x,t) + 6\Upsilon(x,t) - 4\Upsilon(x-\Delta x,t) + \Upsilon(x-2\Delta x,t)] + \sigma(12\Delta t)^{1/2}\nabla\eta(t), \tag{15}$$

where $\sigma = 2D/\Delta x$ and $\eta(t)$ is a random number taken from a Gaussian distribution.

The nonlinear term of LDV equation is discretized as

$$\lambda/2\nabla^3\Upsilon^2 = \lambda/8[\Upsilon^2(x+2\Delta x,t) - 2\Upsilon^2(x+\Delta x,t) + 2\Upsilon^2(x-\Delta x,t) - \Upsilon^2(x-2\Delta x,t)]. \tag{16}$$

Other terms of LDV equation are the same as those of LMBE equation. Then the explicit finite difference approximation of the local derivative of LDV equation (14) can be described as

$$\begin{aligned}\Upsilon(x,t+\Delta t) =& \Upsilon(x,t) + \frac{\sigma}{\Delta x}(12\Delta t)^{1/2}\nabla\eta(t) \\ &- \frac{\nu\Delta t}{(\Delta x)^4}[\Upsilon(x+2\Delta x,t) - 4\Upsilon(x+\Delta x,t) + 6\Upsilon(x,t) - 4\Upsilon(x-\Delta x,t) + \Upsilon(x-2\Delta x,t)] \\ &+ \frac{\lambda\Delta t}{2(\Delta x)^3}[\Upsilon^2(x+2\Delta x,t) - 2\Upsilon^2(x+\Delta x,t) + 2\Upsilon^2(x-\Delta x,t) - \Upsilon^2(x-2\Delta x,t)].\end{aligned} \tag{17}$$

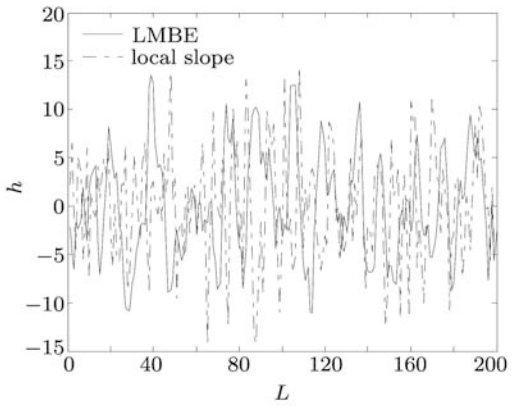


Fig. 1. Comparison between interface profile generated in the $(1+1)$-dimensional LMBE model and its local slope with $L = 200$, and at early time $t = 100$.

We simulate it numerically using a finite-difference method, with choosing the parameters as $\Delta t = 0.05$, $\Delta x = 1$, $\nu = 1$, $\lambda = 0.5$, and $D = 1$, and starting from a flat interface at $t = 0$. Figure 1 shows the typical profiles of the interface generated in the $(1+1)$-dimensional LMBE equation and its local slope with system size $L = 200$, and at early time. In early time regime, LMBE and its local slope have similar interface profiles. When growth time t increases to saturation regime, the mounded morphology appears in LMBE model, however, its local slope still exhibits self-affine surface (see Fig. 2). The existence of grooves instability at saturation (LMBE) is a consequence of the fact that a self-affine surface cannot exist with roughness exponent $\alpha > 1$. This implies that the anomalous behaviour appears to appear in LMBE surface, while its local slope $\Upsilon(x,t)$ as a growing surface still exhibits normal scaling behaviour.

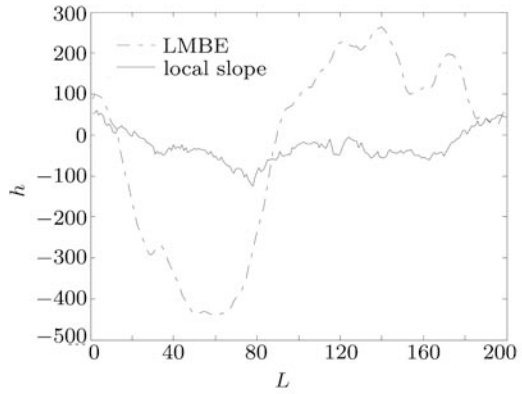


Fig. 2. Comparison between interface profile generated in the (1 + 1)-dimensional LMBE model and its local slope with L=200, and in the saturation time regime, i.e., $t = 10^6$. For the sake of clear comparison, each curve shifts correspondingly along the vertical coordinate.

Figure 3 shows the typical profiles of the interface generated in the (1 + 1)-dimensional LDV equation and its local slope with system size $L = 200$ and in early time regime. At early time, both LDV and its corresponding local derivative can produce symmetric 'hill' and 'valley' patterns. When time t increases to saturation regime, similar to the case of LMBE, the mounded morphology appears in LDV model, however, its local slope still exhibits self-affine character (see Fig. 4). The existence of mounded structure at LDV is a consequence of the fact that a self-affine surface cannot exist with roughness exponent $\alpha = 1$. This implies that the anomalous behaviour appears in LDV growth surface, however, its local slope as a growing surface exhibits standard Family–Vicsek scaling.

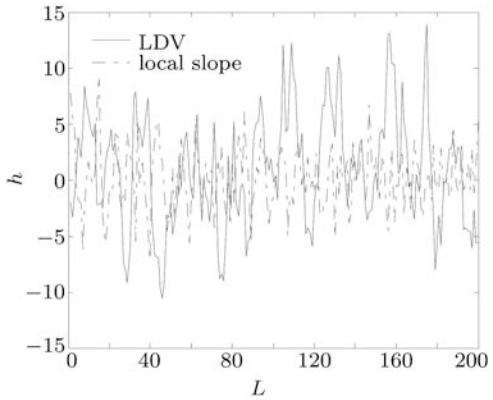


Fig. 3. Typical profiles of the interface generated in the (1 + 1)-dimensional LDV model and local slope with $L = 200$ and at early time $t = 100$.

Figure 5 shows log–log plots of interface width $W(L,t)$ vs. time t for the early regime of LMBE equation and its local slope. The number of samples used for noise averaging is 1000, the substrate size $L = 512$, and the curves are shifted for the sake of clarity. Least square method is used in order to determine the indicated numerical values for β and κ. For the LMBE equation, we obtain the growth exponent $\beta = 0.375 \pm 0.03$ ($\beta = 3/8$ expected), while for its local slope, the anomalous growth exponent $\kappa = 1.25 \pm 0.02$ ($\kappa = 1/8$ expected).

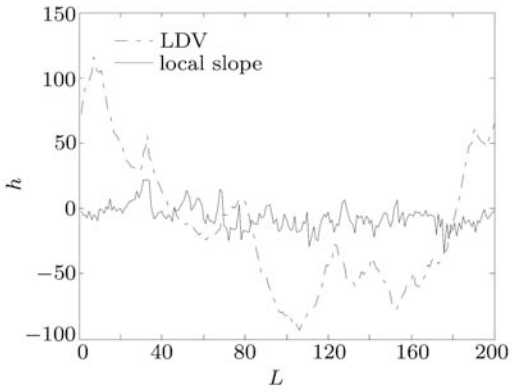


Fig. 4. Typical profiles of the interface generated in the (1 + 1)-dimensional LDV model and local slope with $L = 200$, and in saturation time regime, i.e., $t = 10^6$. For the sake of clear comparison, each curve shifts correspondingly along the vertical coordinate.

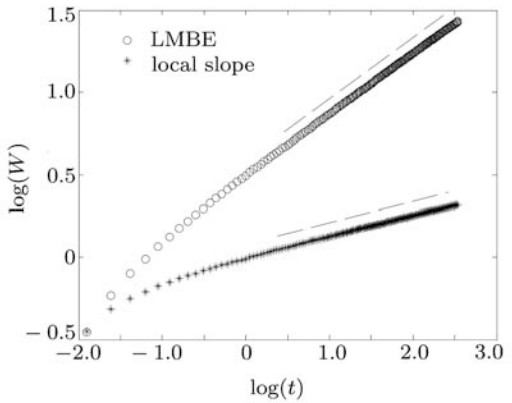


Fig. 5. Log–log plots of width W vs. time t from numerical solution of Eqs. (9) and (10) for system size $L = 512$, and the average is taken over 1000 runs. The circles represent the data for the LMBE equation, while the stars are the date for the local slope of LMBE.

In Fig. 6, log–log plots of $W(L,t)$ versus t is shown for the early regime of LDV and its local slope. We obtain the growth exponent $\beta = 0.34 \pm 0.02$ ($\beta = 1/3$ expected), and the anomalous growth exponent $\kappa = 0.091 \pm 0.03$ ($\kappa = 1/11$ expected). Therefore, the scaling exponent values obtained by simulations from both MBE growth equations and the corresponding local derivatives are in good agreement with

the corresponding analytical predictions mentioned in Section 3.

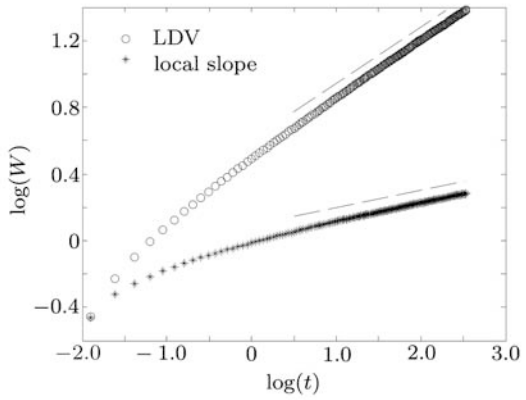


Fig. 6. Log–log plots of width W vs. time t from numerical solution of Eqs. (13) and (14) for system size $L = 512$, and the average is taken over 1000 runs. The circles represent the data for the LDV equation, and the stars denote the date for the local slope of LDV.

5. Conclusions

In this paper, we investigate numerically and analytically anomalous scaling behaviour of MBE growth equation. The anomalous scaling exponents in both the LMBE and LDV equations are obtained based on scaling analysis and finite-difference approximation, respectively. We find the numerical support for the existence of anomalous scaling behaviour in the (1+1)-dimensional MBE growth system. Our numerical results are in good agreement with the corresponding analytical predictions. In addition, we have also discussed the surface formations of MBE growth in early and saturation regimes, separately. The mounded formation in surface growth also provides additional support for the anomalous scaling behaviour of MBE models. Our present work will be helpful for ascertaining the scaling properties of the MBE growth models and investigate the microscopic physical mechanisms of roughness surfaces exhibiting the anomalous scaling behaviour.

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