Numerical study of anomalous dynamic scaling behaviour of (1+1)-dimensional Das Sarma–Tamborenea model*

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In order to discuss the finite-size effect and the anomalous dynamic scaling behaviour of Das Sarma–Tamborenea growth model, the (1+1)-dimensional Das Sarma–Tamborenea model is simulated on a large length scale by using the kinetic Monte–Carlo method. In the simulation, noise reduction technique is used in order to eliminate the crossover effect. Our results show that due to the existence of the finite-size effect, the effective global roughness exponent of the (1+1)-dimensional Das Sarma–Tamborenea model systematically decreases with system size L increasing when $L > 256$. This finding proves the conjecture by Aarao Reis[Aarao Reis F D A 2004 *Phys. Rev.* E **70** 031607]. In addition, our simulation results also show that the Das Sarma–Tamborenea model in 1+1 dimensions indeed exhibits intrinsic anomalous scaling behaviour.

Keywords: finite-size effect, anomalous dynamic scaling, Das Sarma–Tamborenea model, noise reduction technique

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1. Introduction

Many interfaces and surfaces in the nature are examples of self-affine objects. These interfaces and surfaces will appear as kinetic roughening, and exhibit nontrivial scaling property that allows one to divide the growth processes into universality classes.[1−6] This field is significant not only for the study of fundamental problems in nonequilibrium statistical physics and condensed matter physics, but also for practical importance in technological processes and material qualities.

The morphology and the dynamics of a rough surface are usually characterized by global surface width $W(L,t)$, which is defined as

$$W(L,t) = \frac{1}{\sqrt{L}} \left\langle \sum_{\boldsymbol{x}} \left[h(\boldsymbol{x},t) - \bar{h}(t) \right]^2 \right\rangle^{1/2}, \quad (1)$$

where $h(\boldsymbol{x},t)$ is the surface height from a flat substrate of size L at position $\boldsymbol{x}$ and time t, $\bar{h}(t)$ is the mean height of the interface at time t and the angular brackets denote the noise averaging over different realizations. In many cases, starting from an initially flat surface, the global width is observed to satisfy the dynamic scaling formula of Family–Vicsek[7]

$$W(L,t) = t^{\beta} f\left(L/t^{1/z}\right). \quad (2)$$

Scaling function $f(u)$ has an asymptotic property such that $f(u) \sim u^{\alpha}$ for $u \to 0$ and $f(u) \sim$ const. for $u \to \infty$. Roughness exponent α and dynamic exponent z describe the asymptotic behaviour of the growing interface on large length scale and long time scale, and determine the universality class of the model under study. The ratio $\beta = \alpha/z$ is called growth exponent and describes the short time behaviour of the surface. The Family–Vicsek scaling picture has been successfully applied to a great variety of models, which include, for instance, the important universality classes associated with the Edwards–Wilkinson (EW)[8] and Kardar–Parisi–Zhang (KPZ)[9] equations.

However, the Family–Vicsek dynamic scaling for a local width is not guaranteed if the interface is not self-affine, in which case the local and the global surface fluctuations may have different scaling behaviours. This different type of scaling is termed in the literature anomalous scaling and it has been extensively

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investigated.[10−17] For growth process in which an anomalous roughening takes place, the local width or the height–height correlation function scales as

$$w(l,t) \sim \sqrt{G(l,t)} \sim l^{\alpha} f_{\mathrm{A}}(l/t^{1/z}) \tag{3}$$

with an anomalous scaling function

$$f_{\mathrm{A}}(u) \sim \begin{cases} u^{-(\alpha-\alpha_{\mathrm{loc}})} & \text{if} \quad u \ll 1, \\ u^{-\alpha} & \text{if} \quad u \gg 1. \end{cases} \tag{4}$$

This ansatz yields to a different behaviour from that of the Family–Vicsek given in expression (2)

$$w(l,t) \sim \sqrt{G\left(l,t\right)} \sim \begin{cases} l^{\alpha_{\mathrm{loc}}} t^{\beta_*} & \text{if} \quad l \ll t^{1/z}, \\ t^{\beta} & \text{if} \quad l \gg t^{1/z}, \end{cases} \tag{5}$$

with the global (α and β), the local (α_{loc}), and anomalous (β_*) exponents related in the form $\alpha_{\mathrm{loc}} = \alpha\left(1-\beta_*/\beta\right)$. In this case, three exponents, α_{loc} (or β_*), α and β must be considered in order to give a complete description of the scaling behaviour of the surface. The standard self-affine Family–Vicsek scaling is then recovered when $\alpha = \alpha_{\mathrm{loc}}$.

Generally, anomalous scaling is related either to a super-roughening $\alpha > 1$, for which $\alpha_{\mathrm{loc}} = 1$, or to what is termed intrinsic anomalous roughening, characterized by independent local roughness exponent $\alpha_{\mathrm{loc}} < 1$ and global roughness exponent α that may be larger or smaller than 1 but always larger than α_{loc}.[18] The microcosmic physical mechanism that leads to anomalous dynamic scaling and the corresponding theory has been a subject of great interest in recent years.[14−17]

Employ a powerful computer to study discrete models with microcosmic rules reflecting physically important surface processes has achieved a great success in this field.[1,2] From a wide variety of discrete models we focus on the model proposed by Das Sarma and Tamborenea (DT)[19] which is based on the solid-on-solid model of crystal growth and has been designed with growth by molecular-beam epitaxy (MBE). The growth rules of the model (see below) are used to mimic the surface diffusion, the principal mechanism of surface smoothing during MBE. Due to its success in describing the MBE growth process, the DT model has received much attention since it was developed.[20−27] Original simulation of the model[19] in 1+1 dimensions yielded exponents $\alpha = 1.47 \pm 0.1$ and $\beta \approx 0.375 \pm 0.005$. Theoretical investigations[22,23] showed that the dynamic scaling behaviour of the DT growth model can be successfully described by the nonlinear Lai–Das Sarma–Villain (LDV)[28,29] equation

$$\frac{\partial h}{\partial t} = -\kappa \nabla^4 h + \lambda \nabla^2 \left(\nabla h\right)^2 + \eta\left(\boldsymbol{x}, t\right), \tag{6}$$

where the first term on the right-hand side describes the diffusion of a surface by a diffusion coefficient κ,the second term is the nonlinear term describing the lateral growth, and the noise $\eta\left(\boldsymbol{x}, t\right)$ has a Gaussian distribution as

$$\begin{cases} \langle \eta\left(\boldsymbol{x}, t\right) \rangle = 0, \\ \langle \eta\left(\boldsymbol{x}, t\right) \eta\left(\boldsymbol{x}', t'\right) \rangle = 2D\delta\left(\boldsymbol{x}-\boldsymbol{x}'\right)\delta\left(t-t'\right). \end{cases} \tag{7}$$

For the LDV theory, a one-loop dynamic renormalization-group (DRG) calculation[28] leads to $\alpha = 1$, $\beta = 1/3$ in 1+1 dimensions. See also the recent work of Katzav,[30] based on a self-consistent expansion approach, which also obtains these estimates.

Evidently, there exist great differences between the theoretical results of the LDV equation and the simulation results of the DT model. The possible explanation could be a slow crossover effect of the DT model, making the exponents unable to be obtained accurately. In order to eliminate the crossover effects of the DT model, Das Sarma *et al.*[24,25] carried out a numerical calculation on this model by using the noise reduction technique,[31−35] and the scaling exponents $\alpha = 1$ and $\beta = 1/3$ were obtained for system size $L < 100$ in 1+1 dimensions. The calculation result given by Das Sarma *et al.* is consistent with the theoretical analysis of the LDV equation. Based on the work by Das Sarma and coworkers,[24,25] Aarao Reis[27] extended the system size up to $L = 256$ so as to obtain the scaling behaviour of the (1+1)-dimensional DT model on a large length scale. However, the simulation results show that the global roughness exponent is larger than 1 and systematically increases with L increasing. Although the (1+1)-dimensional DT model for $L > 256$ was not simulated, Aarao Reis[27] made the conjecture that, due to the finite-size effect, the effective global roughness exponents for the noise-reduced DT model would eventually begin to decrease with L increasing, possibly for much larger values of L. To the best of our knowledge, the conjecture by Aarao Reis has not been proved yet. So the investigating of the influence of finite-size effect on the scaling behaviour of the DT model on large length scale in order to prove the conjecture by Aarao Reis is one of our motivations in the paper.

In addition, it is important to note that anomalous scaling stems from the fact that the mean square local slope has nontrivial dynamics.[36] A standard (Family–Vicsek) self-affine scaling of the local interface fluctuations, i.e. $\alpha = \alpha_{\rm loc}$, implies that the square local slope $G\,(l = a, t) = \left\langle [h(\boldsymbol{x} + \boldsymbol{a}, t) - h(\boldsymbol{x}, t)]^2 \right\rangle$, where a is the lattice spacing, becomes $G(a, t) \sim$ const. very rapidly in time. However, in growth models exhibiting anomalous scaling the local slopes scale as $G(a, t) \sim t^{2\beta_*}$.[36] The existence of such a diverging means that the local slope introduces a new correlation length in the growth direction, which enters the scaling of the local fluctuations of the height. Therefore, in any growth model, the existence (or absence) of anomalous scaling of the local height fluctuations can be investigated by computing the mean local slope $G(a, t)$. This method is illustrated by studying several growth equations with and without anomalous scaling by using the scaling approach,[36,37] and the results show that the LDV equation in 1+1 dimensions exhibits intrinsic anomalous scaling behaviour in the strong coupling region with $\beta_* = 1/11$. It is a valuable work to ascertain the anomalous scaling behaviour of the DT model and investigate the microcosmic physical mechanism of anomalous dynamic scaling.

As mentioned above, our work of simulating the DT model in 1+1 dimensions on large length scale is useful to prove the conjecture given by Aarao Reis and investigate the anomalous scaling behaviour of this model.

In the paper, the (1+1)-dimensional DT growth model is simulated on large length scale by using the noise reduction technique. We extend the system size to sites as large as $L = 1024$ and deposition time up to 2^{27} layers. The global growth exponent $\beta = 0.334 \pm 0.002$ is obtained by calculating the global width, and the result is consistent with the theoretical analysis of the LDV equation. Our calculation results of global width also show that the effective global roughness exponent increases with the system size L increasing when $L < 256$, whose behaviour was also found by Aarao Reis.[27] However, when $L > 256$, the effective global roughness exponent turns to decrease with L increasing. This finding proves the conjecture given by Aarao Reis. In addition, it is found that the scaling behaviour of the local width is different from that of the global width, and $\beta_* = 0.092 \pm 0.003$ is obtained. The result shows that the (1+1)-dimensional DT model exhibits intrinsic anomalous scaling. This conclusion reproduces the analytical result of the LDV equation in the strong coupling region by using the scaling approach, so the intrinsic anomalous scaling behaviour of the (1+1)-dimensional DT model is consistent with that obtained from the LDV equation in the strong coupling region.

The rest of the present paper is organized as follows. In Section 2, we introduce the basic algorithm for the noise reduction technique. Section 3 contains our simulation results and discussions. The conclusions are given in Section 4.

2. Noise reduction technique

In the simulation of the (1+1)-dimensional DT model, the noise reduction technique[24,25,31–35] is used to eliminate the slow crossover effects.

The idea behind the noise reduction technique is that noise induces large hills and valleys on the growing surface which hinder the accurate measuring of the scaling exponents, and consequently any technique that suppresses large hills and valleys (i.e., large nearest-neighbour height differences) should lead to a better scaling behaviour and relatively accurate estimate of the scaling exponent. The noise reduction technique, which has been very successful in suppressing corrections to the scaling in several different nonequilibrium growth processes (e.g. diffusion-limited aggregation, Eden growth, ballistic deposition), achieves a good scaling behaviour[32–35] (and consequently a better critical exponent) by accepting only a small fraction (to be precise, a fraction of $1/m$, where $m > 1$ is the noise reduction factor) of the incident particles and thereby greatly suppressing large hills and valleys in the noise-reduction growth morphology.

The basic algorithm[24,25] for the noise reduction technique involves putting a virtual counter on each surface lattice site to register a positive count m every time a new atom from the incident beam randomly drops on that counter. A real deposition event is allowed in the simulation only when the counter registers a predetermined value of m (for example, $m = 5$ or 10, etc.). No actual deposition or incorporation occurs at that particular site until m reaches a predetermined noise reduction number (which, of course, holds true for each surface site). For $m = 1$, a noise reduction factor of unity, the growth model by definition is the same as the usual growth simulation without any noise reduction. Note that a large value of the noise

reduction parameter m does not conduce to the situation because it suppresses kinetic surface roughening far too well from producing smooth layer-by-layer growth with essentially no roughening. The optimal value of m has to be chosen by trial and error for specific growth models—m cannot be too small, for noise effects will then dominate with steep hills and deep valleys (large values of surface height gradients), and m cannot be too large since the smooth layer-by-layer growth will then proceed indefinitely with no kinetic surface roughening.

It has been shown that the noise reduction technique does not modify the universality class of a growth model.[31−35]

3. Simulation results and discussion

3.1. Das Sarma–Tamborenea model

The growth rules of (1+1)-dimensional DT model are shown in Fig. 1. In this model, the incident particle sticks at the top of the randomly chosen column i if it has one or two lateral neighbours at that position (a kink site or a valley, respectively). Otherwise, the neighbouring columns (on the right and the left sides in 1+1 dimensions) are consulted. If the top position of only one of these columns is a kink site or a valley, then the incident particle aggregates at that point. If no neighbouring column satisfies that condition, then the particle sticks at the top of column i. Finally, if both neighbouring columns satisfy that condition, then one of them is randomly chosen.

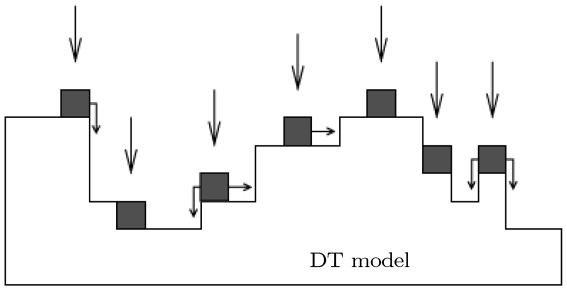


Fig. 1. Growth rules of (1+1)-dimensional Das Sarma-Tamborenea (DT) model given by Ref.[26].

The DT growth model successfully describes the MBE growth process, so it has received much attention.[20−27]

3.2. Dynamic scaling behaviour of global width

In 1+1 dimensions, we carried out simulations for different lattice sizes: $L = 32$, 64, 128, 256, 512, and 1024 with periodic boundary conditions in the direction of the substrate. All our calculations are results of extensive averaging over many simulation runs (the number of runs up to the steady state is typically 10^4 for the smallest lattices and nearly 200 for the largest lattices, and each run is self-averaging since we average over all the substrate lattice sizes). During the simulations, a time unit corresponds to the deposition of L particles. We use $m = 10$ for the results shown in this paper, because it provided accurate estimates of scaling exponents in Refs. [24], [25], and [27].

Figure 2 shows the curves for global width W versus growth time t for different system sizes. It can be seen clearly from Fig. 2 that the global width of the DT model is independent of the system size at the beginning phase, and independent of the growth time at saturated phase. Global growth exponent $\beta = 0.334 \pm 0.002$ is obtained by using the initial slope of the global width for $L = 1024$ as shown in Fig. 2, and this result is consistent with the analytical result of the (1+1)-dimensional LDV equation.

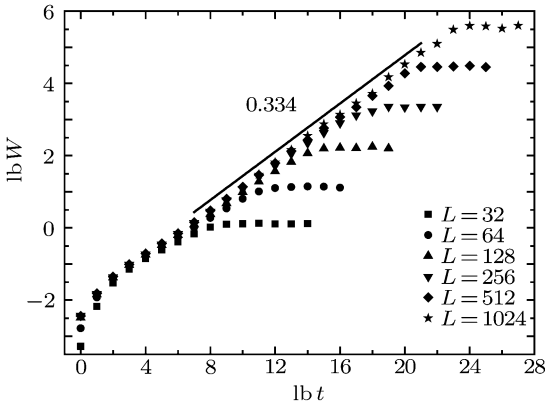


Fig. 2. Curves for Log–log plot of global width W versus growth time t for different system sizes.

Due to the existence of finite-size effect in the DT model, global roughness exponent α cannot be obtained in a high accuracy just from the relation $W_{\rm sat}(L,t) \sim L^{\alpha}$ ($W_{\rm sat}$ is the global width in the steady state) for different values of L. Here systematic extrapolations of effective global roughness exponents for the DT model are performed.

Since reliable estimates of the interface width at the steady state ($W_{\rm sat}$) are needed, the first step is to

compute that quantity in various time ranges, in order to find a region in which W is fluctuating around an average value. Then a final estimate of $W_{\rm sat}$ is performed. Finite-size estimate of the exponent α is given by[27]

$$\alpha_L = \frac{\ln[W_{\rm sat}(L)/W_{\rm sat}(L/2)]}{\ln 2}, \tag{8}$$

which we expect to converge into an asymptotic value as $L \to \infty$.

In Fig. 3, we show effective roughness exponent α_L as a function of L for the noise-reduced DT model. It is larger than $\alpha = 1$ and systematically increases with L increasing when $L < 256$. The result in this region is also obtained in the simulation work by Aarao Reis.[27] However, when $L > 256$, it shows a continuous decrease of the effective roughness exponent, which proves the conjecture by Aarao Reis (for 'it is expected that the effective exponents for the noise-reduced DT model will eventually begin to decrease with L, possibly for much larger L'.[27]) It can also be seen from Fig. 3 that the effective roughness exponent comes to a maximal value near $L = 256$, so we come to the conclusion that the finite-size effect of the noise-reduced DT model is more prominent near $L = 256$. Performing extrapolations of the effective global roughness exponents, the second-degree curve gives $\alpha \approx 1.01$ when $L \to \infty$.

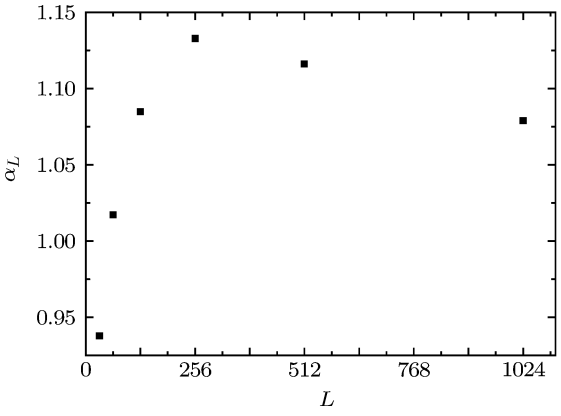


Fig. 3. Effective roughness exponent α_L versus L for the noise-reduced DT model.

The global dynamic scaling exponents of the (1+1)-dimensional DT model are obtained by calculating the global width in this subsection, and the results here are in agreement with the analytical conclusion.[28] We can also see that the noise reduction technique can effectively eliminate crossover effects, enabling us to obtain better scaling behaviour even when the system size is not very large.

3.3. Dynamic scaling behaviour of local width

Anomalous scaling implies that one more independent exponent may be needed in order to assess the universality class of the particular system under study. In other words, some growth models may have exactly the same α and β values, seemingly indicating that they belong to the same universality class. However, they may have different values of local exponent, showing that they actually belong to distinct classes of growth. So the local scaling behaviour of the (1+1)-dimensional DT model must be considered.

Local scaling exponent of the (1+1)-dimensional DT model is calculated by analysing the local width, and the plots of lb$w$ versus lb$t$ for $L = 256$ and $L = 512$ are shown in Figs. 4 and 5, respectively.

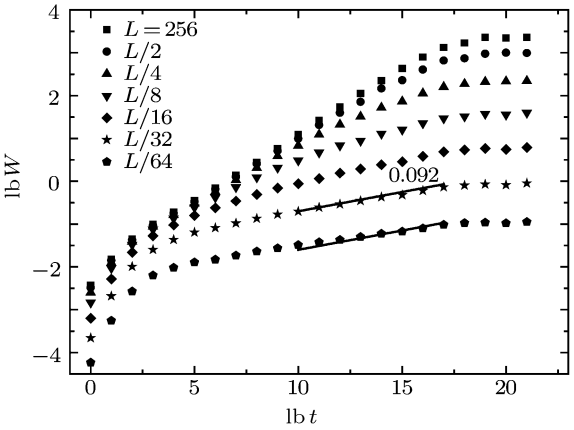


Fig. 4. Log–log plots of local width w versus growth time t, $L = 256$.

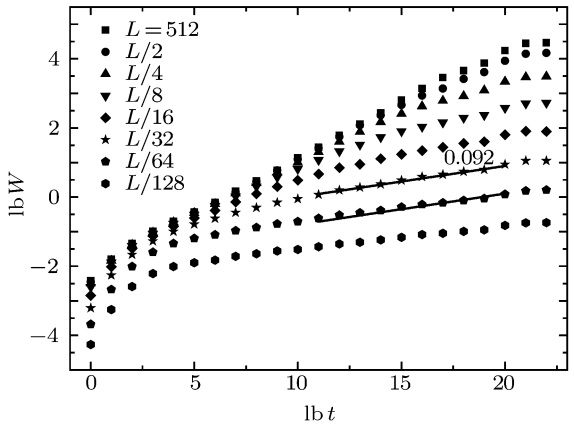


Fig. 5. Log–log plots of local width w versus growth time t, $L = 512$.

In Fig. 4, each curve corresponds to the surface height fluctuation over a window of size l from system size $L = 256$. For each size l, local width w saturates at $t \sim L^z$, which is the same saturated time as global

width W. This means that the local and the global surface fluctuations have different scaling behaviours (if the local and the global surface fluctuations have the same scaling behaviours, then the saturated time for each l should be $t \sim l^z$, rather than $t \sim L^z$). The different scaling behaviours of the local and the global widths show that the DT model in 1+1 dimensions exhibits anomalous scaling. For $l = L/32$ and $l = L/64$, two curves have the same slopes in the growth region, and the local growth exponent can be obtained.

The analytical procedure of Fig. 4 can also be used for Fig. 5, and local growth exponent $\beta_* = 0.092 \pm 0.003$ is obtained and shown in Fig. 5.

The local growth exponent obtained from the local width differs substantially from the value of global exponents ($\beta = 0.334 \pm 0.002$ and $\alpha \approx 1.01$) obtained from the global width, which indicates that the DT model in 1+1 dimensions exhibits intrinsic anomalous scaling. This conclusion is consistent with the recent theoretical analysis of the (1+1)-dimensional LDV equation in the strong coupling region based on a scaling approach.[36,37]

The exhibition of the intrinsic anomalous scaling behaviour here is due to the fact that the surface of the DT model in 1+1 dimensions is not self-affine. An interesting fact should be stressed that the equality $\alpha_{\rm loc} = \alpha$ (or $\beta_* = \beta$) is not guaranteed in general when Family–Vicsek scaling holds for the global width, since the self-affinity of the interface and the surface is an additional independent conditions.[18] The existence of dynamic scaling as shown in expression (2) under the assumption of the self-affine character of the surface—in the sense that there is no characteristic length scale in the surface besides the system size, and therefore all scales obey the same physics—allows one to obtain the exponent from local width $w(l, t)$, and the local width has the same scaling behaviour as the global width. However, when the surface is not self-affine, the local and the global widths have distinctly different scaling behaviours. This leads to the existence of an independent local scaling exponent that is characterized by the local interface fluctuations and differs from the global scaling exponent, and the model under study exhibits an anomalous scaling behaviour.

4. Conclusions

The (1+1)-dimensional DT model is simulated on a large length scale. The noise reduction technique is employed so as to eliminate crossover effects. The global width and the local width are calculated separately. Global growth exponent $\beta = 0.334 \pm 0.002$ is obtained by calculating the global width, and the result is consistent with the theoretical analysis of LDV equation. The calculation results of global width also show that due to the existence of the finite-size effect, the effective global roughness exponent of (1+1)-dimensional DT model first increases with system size L increasing, and then decreases with size increasing when $L > 256$. In addition, it is found that the scaling behaviour of the local width is different from that of the global width, and $\beta_* = 0.092 \pm 0.003$ is obtained. The result shows that the (1+1)-dimensional DT model exhibits intrinsic anomalous scaling behaviour which is in good agreement with the scaling behaviour of the LDV equation in the strong coupling region.[36,37]

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