Physica A 471 (2017) 569–575

Contents lists available at ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

Influences of large height differences and overhangs on the dynamic scaling behavior of discrete models

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HIGHLIGHTS

- The Etching model is improved to reduce large height differences.
- The overhangs in the Ballistic Deposition model are removed.
- Modified surfaces lead to good dynamic scaling behavior even on small systems.

ARTICLE INFO

Article history:
Received 18 February 2016
Received in revised form 4 September 2016
Available online 24 December 2016

Keywords:
Large height differences
Overhangs
Dynamic scaling
Discrete model

ABSTRACT

In order to investigate the influences of large height differences and overhangs on the dynamic scaling behavior of discrete models, meanwhile reducing the finite-size effects, the Etching model is modified to reduce large height differences, and the overhangs in Ballistic Deposition surfaces are removed under certain principles. Numerical simulations are carried out for the modified models, and the results show that the modified surfaces lead to good dynamic scaling behavior even on small system length scales. The values of the dynamic scaling exponents are in excellent agreement with theoretical predictions of the Kardar–Parisi–Zhang equation in $(1 + 1)$ dimensions.

1. Introduction

Fluctuating surfaces and interfaces are among the most highly studied non-equilibrium systems due to their simplicity as well as numerous practical applications in processes such as crystal growth, erosion, and material fracture. Thereby, in the past two decades, physicists in the statistical physics and condensed matter physics community have devoted considerable efforts by both experimental and theoretical (analytical and numerical) ways and many valuable achievements have been achieved so far [1–4].

Surfaces and interfaces can exhibit kinetic roughening phenomena. A quantitative description of the roughness dynamics of surfaces and interfaces is based on scaling laws for the correlation lengths of the system, which reflect the scale invariance of the problem. Those scaling properties introduce a series of scaling exponents that do not depend on the particular details of the model thus allowing a classification of different types of surface growth into universality classes. More precisely, the dynamics of a rough surface are usually characterized by the global surface width $W(L, t)$, which is defined as

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

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http://dx.doi.org/10.1016/j.physa.2016.12.042

where $h(\mathbf{x}, t)$ is the surface height from a flat substrate of size L at position $\mathbf{x}$ 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 form of Family–Vicsek [5]

$$W(L, t) = t^{\beta} f(L/t^{1/z}), \tag{2}$$

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

$$f(u) \sim \begin{cases} u^{\alpha}, & \text{if} \quad u \ll 1 \\ \text{const}, & \text{if} \quad u \gg 1. \end{cases} \tag{3}$$

The roughness exponent α and dynamic exponent z describe the asymptotic behavior of the growing interface on large length 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 behavior of the surface.

Surface growth phenomena can be categorized into various universality classes [1,2]. The most prominent and well-known one of them is the Kardar–Parisi–Zhang (KPZ) [6] class, for which the growth can be described by a continuum equation, given as

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

The first term on the right hand side describes the relaxation of interface caused by a surface tension ν, and the second term reflects the presence of lateral growth with the coefficient λ. η is the Gaussian random variable which satisfies

$$\langle \eta (\mathbf{x}, t) \eta \left(\mathbf{x}', t'\right) \rangle = 2D\delta \left(\boldsymbol{x} - \boldsymbol{x}'\right) \delta \left(t - t'\right), \tag{5}$$

with D describing the strength of the noise. As a diffusive Langevin equation supplemented by rotationally invariant nonlinearity, the KPZ equation has become a fundamental equation. Many researchers have focused on investigating the properties of this equation, or the corresponding experiments [6–20]. Because of the nonlinearity of the equation, exact analytic solution has been a tough work, especially in $(2 + 1)$ dimensions. Theoretical methods [6–8] give exact results $\alpha = 1/2$, $\beta = 1/3$ in $(1 + 1)$ dimensions. In higher dimensions, however, we have only the scaling relation $\alpha + z = 2$.

Due to their success in the investigation of the physical mechanism and morphology properties of the kinetic roughening of surfaces and interfaces, the discrete growth theory was widely used. Many microscopic growth models were introduced to mimic different practical growth processes. By discussing the symmetries and conservation laws of the model obeying in the growth process, the corresponding continuum equation, or universality class, can be obtained. Models can be described by the same continuum equation are believed to belong to the same universality class. It is shown that the Ballistic Deposition (BD) model [21,22], the Etching model [23], and the Restricted solid-on-solid (RSOS) model [24] can be described by the KPZ equation (i.e., belong to the KPZ universality class).

These discrete models play an important role in the investigations of kinetic roughening of surface and interfaces and the scaling properties of the corresponding equations, and many meaningful results have been achieved [21–37]. However, there are still some flaws. Firstly, the existence of overhangs and voids in BD model leads to obvious finite size effects, and hinder the asymptotic scaling of this model in small systems. So numerical simulations must be carried out on very large length and long time scales (which is also time consuming), or some correction methods, such as the system extrapolation method proposed by Aarao Reis [27], have to be employed. Until 2011 [31], extensive kinetic Monte Carlo simulations were presented for BD model in $(1+1)$ dimensions on very large system sizes, and the asymptotic scaling of this model was found for lattice sizes $L \geq 2^{12}$. In addition, because of the existence of large height differences in the surfaces, similar situation can be found in the Etching model [23].

In this paper, in order to reduce finite size effects, at the same time, investigate the influences of large height differences and overhangs on the dynamic scaling behavior of discrete models, the Etching model is modified to reduce large height differences, and the overhangs in BD surfaces are removed. All these operations do not change the symmetries of the models. Simulation results show that large height differences and overhangs indeed obviously affect the scaling behavior of the models, and modified models lead to good dynamic scaling (very weak finite size effects) on small system scales. The scaling exponents $\alpha = 0.500 \pm 0.001$, $\beta = 0.332 \pm 0.001$ are calculated for modified Etching model, and $\alpha = 0.500 \pm 0.002$ is estimated for BD model without overhangs. These results are consistent with the theoretical analysis of the KPZ equation in $(1 + 1)$ dimensions.

The rest of the paper is organized as follows. The dynamic scaling behavior of the modified Etching model and BD model after removing the overhangs are discussed in Sections 2 and 3, respectively. In the last section, i.e., Section 4, we present our conclusions.

2. Dynamic scaling of modified Etching model

The Etching model was proposed to describe dissolution of a crystalline solid by a liquid. Assuming that the substrate is a square lattice with a one-dimensional surface exposed to dissolution, the cellular automata algorithm (in its growth version) that simulates the model in $(1 + 1)$ dimensions is