Physica B 405 (2010) 2072–2077

Contents lists available at ScienceDirect

Physica B

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

Solid-on-solid model for surface growth in 2+1 dimensions

S. Hosseinabadi [a], A.A. Masoudi [a,b,*], M. Sadegh Movahed [c]

[a] Department of Physics, Alzahra University, P.O. Box 19938, Tehran 91167, Iran
[b] Department of Applied Mathematics, University of Waterloo, Waterloo, ON, Canada N2L 3G1
[c] Department of Physics, Shahid Beheshti University, G.C., Evin, Tehran 19839, Iran

A R T I C L E I N F O

Article history:
Received 13 November 2009
Received in revised form
18 January 2010
Accepted 19 January 2010

Keywords:
Surface growth
Scaling exponents

A B S T R A C T

We analyze in detail the solid-on-solid (SOS) model for growth processes on a square substrate in 2+1 dimensions. By using the Markovian surface properties, we introduce an alternative approach for determining the roughness exponent of a special type of SOS model—the restricted-solid-on-solid (RSOS) model—in 2+1 dimensions. This model is the SOS model with the additional restriction that the height difference must be S=1. Our numerical results show that the behavior of the SOS model in 2+1 dimensions for approximately $S \geq S_{\times} \sim 8$ belongs to the two different universality classes: during the initial time stage, $t < t_{\times}$ it belongs to the random-deposition (RD) class, while for $t_{\times} < t \ll t_{sat}$ it belongs to the Kardar–Parisi–Zhang (KPZ) universality class. The crossover time ($t_{\times}$) is related to S via a power law with exponent, $\eta = 1.99 \pm 0.02$ at 1σ confidence level which is the same as that for 1+1 dimensions reported in Chein and Pang (2004) [8]. Using the structure function, we compute the roughness exponent. In contrast to the growth exponent, the roughness exponent does not show crossover for different values of S. The scaling exponents of the structure function for fixed values of separation distance versus S in one and two space dimensions are $\xi = 0.92 \pm 0.05$ and $\xi = 0.86 \pm 0.05$ at 1σ confidence level, respectively.

1. Introduction

Surface growth processes, especially the formation of thin film deposits, have been studied using various approaches in complex systems and statistical analysis [1–7]. The factors which control surface growth phenomena have immense phase space. Consequently, to be able to analyze these phenomena one needs to make many assumptions, which can lead to results that are unreliable. Combining insights from computational simulation and simplified analysis will likely give better results. It is well known that the understanding of phenomena such as advances of bacterial colonies, electrochemical deposition, flameless fire fronts and molecular-beam-epitaxial growth is of considerable importance in the control of many interesting growth processes in industries [7–9]. The simplest surface growth model is the so-called statistical deposition model [7,10]. Some models proposed to explore growth surfaces, such as the Family model [11], ballistic deposition (BD) model [12,13] and Eden model [14], are able to account for many of the properties of some real systems. For example, the BD and Eden models can accurately simulate vapor deposition and biological growth. However, these models tend to ignore the microscopic details of the interfaces, and cannot provide accurate scaling exponents. In addition many fractal features of real systems remain unexplained [9,15,16]. To solve these problems, one should modify the above models.

The solid-on-solid (SOS) model is more suitable to describe a real surface's properties than those models described above [8,17–19]. This growth model does not exhibit strong corrections to scaling and consequently allows us to determine accurate values of scaling exponents [7,17,18]. The restricted-solid-on-solid (RSOS) model (a modified version of the SOS model), proposed by Kim et al. [17], is most important due to its wide applicability, such as for surface roughening modeling via exothermic catalytic reactions on the substrate [8]. Various aspects of the solid-on-solid model for surface growth have been studied: the effect of long-range elastic interactions [20], growth processes with correlated noise [21], phase transitions as a function of temperature-like parameters [22], the (0 0 1)-surface morphology of GaAs annealed at fixed temperature and pressure, the well explained by annealed version of the RSOS model [23,24]. Crossover from random to correlated regime [25,26], relaxation to steady states [27], distribution of local configurations for finite values of S [8], Markov analysis [28], the effect of hopping in various local growth rules on the linear and nonlinear fourth-order dynamical growth equation [29], growth model in higher dimensions [30] and, more recently, the growth on fractal

* Corresponding author at: Department of Applied Mathematics, University of Waterloo, Waterloo, ON, Canada N2L 3G1. Tel.: +1 519 888 4567.
E-mail address: amasoudi@math.uwaterloo.ca (A.A. Masoudi).

0921-4526/$ - see front matter © 2010 Elsevier B.V. All rights reserved.
doi:10.1016/j.physb.2010.01.105

substrates based on the SOS model [31], has also been addressed in the literature.

As mentioned in many previous studies, it is believed that the RSOS model belongs to the Kardar–Parisi–Zhang (KPZ) universality class in the continuum limit [32,33]. The KPZ equation is one of the most important phenomenological theories in which time evolution of the interface has been characterized by the height function $h(\vec{r},t)$ at position $\vec{r}$ and time t. The governing equation is given by [34]

$$\frac{\partial h(\vec{r},t)}{\partial t} = \nu \nabla^2 h(\vec{r},t) + \frac{\lambda}{2}[\nabla h(\vec{r},t)]^2 + K(\vec{r},t). \tag{1}$$

Here ν and λ represent the surface tension and the excess velocity respectively, while $K(\vec{r},t)$ is a Gaussian noise with zero mean and co-variance $\langle K(\vec{r},t)K(\vec{r}',t')\rangle = D\delta^d(\vec{r}-\vec{r}')\delta(t-t')$ where d is the dimension of the substrate, and D is the noise intensity [7,12]. The interface width reads as

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

This characterizes the roughness of the interface, for growth in a substrate of length L, and $\overline{h}(t)$ is the spatial average of height at time t. For short times, the interface scales as follows:

$$W(L,t) \approx t^{\beta}, \tag{3}$$

where β is called the growth exponent. For long times, a steady state is attained and the width is saturated as follows:

$$W_{sat}(L,t) \approx L^{\alpha}. \tag{4}$$

Here α is the roughness exponent. Eqs. (3) and (4) correspond to limits of the dynamical relation of the Family and Vicsek ansatz:

$$W(L,t) \approx L^{\alpha} f\left(\frac{t}{L^z}\right). \tag{5}$$

The dynamical exponent, $z=\alpha/\beta$, characterizes the crossover from the growth regime to the steady state. The exact scaling exponents are known in d=1, but no exact value has been obtained in two or more dimensions [16]. Many discrete models fall into the KPZ class, such as the RSOS model [17,18] and ballistic deposition (BD) [12]. Most of the reported values of α range from 0.37 to 0.40 [17,18,35–37], confirmed by numerical solutions of the KPZ equation [38–40].

The competition between different growth mechanisms during particle deposition, as well as phase transitions which are very often observed in many real growth processes, has been investigated in many studies [25,26]. Recently, it has been confirmed that there exists a crossover between the random deposition and KPZ classes at the initial growth stages for all values of the height restriction parameter between nearest neighbors for the SOS model in 1+1 dimension [8]. Here we are interested in investigating the possibility of the existence of crossover in the SOS model in 2+1 dimensions. In addition, we give a new approach to determine the roughness exponent using Markovian properties of surfaces.

The rest of this paper is organized as follows: in Section 2, we introduce the Markovian surface, and by using the characteristic function, the roughness exponent is calculated. The SOS model for finite values of S is numerically investigated in Section 3. Crossover in the growth mechanism and corresponding properties are also investigated in detail in Section 3. Section 4 is devoted to conclusions and summary of our studies.

2. Markovian surface

The Markovian surface is one of several models to represent multi-level (stepped) crystalline surfaces. In this model, it is assumed that the steps have only a mono-atomic height. Displacement through any steps may be *upward* or *downward*, each occurring with equal probability. Let γ be the probability of meeting an atom displaced vertically either upward or downward in going from any lattice site to an adjacent one. That is, the probability of encountering a step ($\Delta h = \pm 1$) while the corresponding probability for a lateral walk, namely $\Delta h = 0$ (h is the height of the surface), is equal to $1-\gamma$. Since every displacement or step occurs independent of any other, the step surface is mapped to the path of a Markovian chain [41]. For the Markovian chain or random walk model, there exist three choices for the displacement at each walk: an upward walk with a probability $\gamma/2$, a downward walk with a probability $\gamma/2$ and a lateral walk with a probability $1-\gamma$ [41]. As mentioned in the introduction, here we rely on the Markovian surface to explore the scaling exponent of the RSOS growth model. To this end, we introduce the characteristic function defined as the Fourier transform of the probability distribution function, $P(\Delta h(\vec{r}))$, with respect to $\Delta h(\vec{r}) = h(\vec{r}) - h(0)$ after saturation time, as

$$Z_d(\lambda,\vec{r}) = \langle e^{i\lambda c[h(\vec{r})-h(0)]}\rangle, \tag{6}$$

where c is the unit of step variations, which is equal to one in the Markovian surface and RSOS model. The height difference, $h(\vec{r})-h(0)$ can be represented as the sum of the height differences between successive sites from r=0 to r=na in one dimension and to $r=\sqrt{(n_x^2+n_y^2)}a$ in two dimensions (a is lattice unit). In one dimension we have [41]

$$h(na)-h(0) = \sum_{i=1}^{n}[h(ia)-h((i-1)a)]. \tag{7}$$

For the RSOS model in 2+1 dimensions, the height difference between any sites with coordinates (n_x,n_y) and its nearest neighbor sites with coordinates $(n_x \pm 1, n_y)$ and $(n_x, n_y \pm 1)$ is ± 1. To calculate the characteristic function, we should move from point $\vec{r}=(0,0)$ to $\vec{r}=(n_x,n_y)$ in different paths like path A as shown in Fig. 1. So the vector sum of the trajectories within path A gives the vector $\vec{r}$. Due to isotropy and homogeneity of the

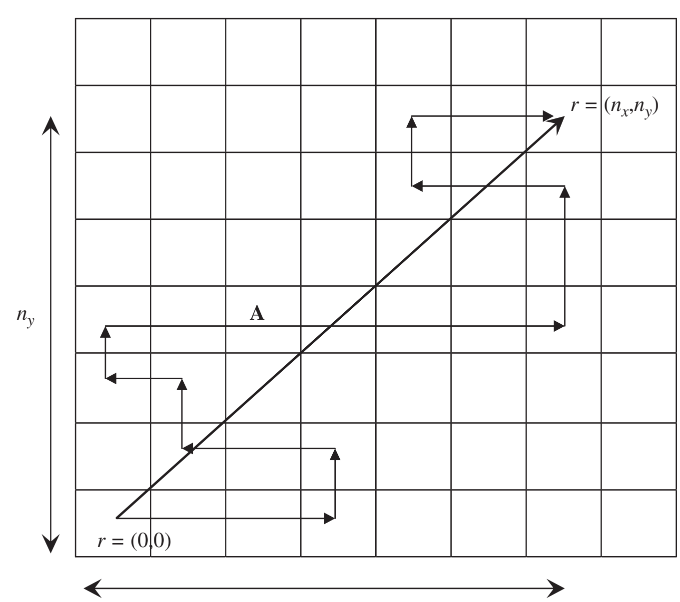

Fig. 1. A typical trajectory from point r=(0,0) to r= (n_x,n_y).