Physica A 493 (2018) 135–147

Contents lists available at ScienceDirect

Physica A

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

Thin film growth by 3D multi-particle diffusion limited aggregation model: Anomalous roughening and fractal analysis

Maryam Nasehnejad, G. Nabiyouni, Mehran Gholipour Shahraki *

Department of Physics, Faculty of Science, Arak University, Arak 38156-8-8349, Iran

HIGHLIGHTS

- A 3D multi-particle diffusion limited aggregation method is employed to simulate growth of rough surfaces in electrodeposition process.
- The simulated surfaces exhibit a complex behavior which is called as anomalous scaling.
- The values of H and β that have been measured by this model are close to KPZ universality class.
- A dynamic scaling ansatz is suggested for interface width as a function of thickness, scan length and probability P.
- The values of $H = 0.45$, $\beta_{loc} = 0.46$, $\beta = 0.35$, $(H/\beta) = 1.29$, $\delta = 0.16$, $\gamma = 0.14$ and $y = 0.05$ are found for characteristic scaling exponents.

ARTICLE INFO

Article history:
Received 15 February 2017
Received in revised form 17 August 2017

Keywords:
Electrodeposition
Multi-particle diffusion limited aggregation (DLA) model
Surface roughness
Fractal dimension
Anomalous scaling

ABSTRACT

In this study a 3D multi-particle diffusion limited aggregation method is employed to simulate growth of rough surfaces with fractal behavior in electrodeposition process. A deposition model is used in which the radial motion of the particles with probability P, competes with random motions with probability $1 - P$. Thin films growth is simulated for different values of probability P (related to the electric field) and thickness of the layer(related to the number of deposited particles). The influence of these parameters on morphology, kinetic of roughening and the fractal dimension of the simulated surfaces has been investigated. The results show that the surface roughness increases with increasing the deposition time and scaling exponents exhibit a complex behavior which is called as anomalous scaling. It seems that in electrodeposition process, radial motion of the particles toward the growing seeds may be an important mechanism leading to anomalous scaling.

The results also indicate that the larger values of probability P, results in smoother topography with more densely packed structure. We have suggested a dynamic scaling ansatz for interface width has a function of deposition time, scan length and probability. Two different methods are employed to evaluate the fractal dimension of the simulated surfaces which are "cube counting" and "roughness" methods. The results of both methods show that by increasing the probability P or decreasing the deposition time, the fractal

* Corresponding author.
E-mail address: m-gholipour@araku.ac.ir (M. Gholipour Shahraki).

https://doi.org/10.1016/j.physa.2017.09.099
0378-4371/

dimension of the simulated surfaces is increased. All gained values for fractal dimensions are close to 2.5 in the diffusion limited aggregation model.

1. Introduction

Non-equilibrium physics is associated with problems that exact balance condition is not satisfied or a Hamiltonian formulation is not possible for them. The growth of thin films by different techniques such as chemical deposition, vapor deposition, electro-deposition and etc. is an example of these problems. Generally, existence of non-equilibrium processes during growth of thin films leads to formation of rough surfaces. Roughness is a well-known quantitative and measurable characteristic of surface which describes surface irregularities. Understanding the behavior of surface roughness during growth process can help us to control electrical [1], optical [2,3], mechanical [4], catalytic [5] and magnetic [6] properties of thin films. It can also enable us to study the important parameters in producing a surface [7–9]. Therefore, development and production of thin film devices with technological applications requires knowledge about the essential mechanisms that affect surface growth. This motivates the study of discrete and continuous growth models and kinetic roughening theories. In this way dominant factors which affect the dynamic processes such as surface diffusion, absorption and reaction have been studied [10,11]. In many of cases, fluctuations of surface follow the Family–Vicsek phenomenological scaling approach where global and local surface fluctuations scale with the same exponents. This is known as normal roughening [8,12]. On the other hand, if local exponents and global exponents are different and local slopes continuously increase, the system shows anomalous roughening [13,14].

Growth and roughness evolution of surface is a non-stationary random process [15,16], which can be identified by some statistical parameters such as standard deviation, slope and curvature of the surface height [17]. Studies have proved that different surfaces, exhibit different roughness on different length scales [18,19].

Due to multi-scale nature of surface roughness, these statistical parameters depend on the length scale. Thus, they are not unique even for a particular surface. Therefore, it is necessary to employ scale-independent parameters for surface characterization. Majumdar et al. [18,20] have demonstrated that the multi-scale nature of surface roughness can be described by fractal geometry [21]. Fractal approach has the ability to characterize a rough surface using scale-independent parameters such as fractal dimension. Fractal dimension is a characteristic which shows how an object fills the space. It also can be used to describe surface topography. An important feature of fractal dimension is the ability to describe complexity of a surface with a number [22,23]. Many of experimental reports show that fractal dimension is associated with surface roughness parameters [24–26]. For each surface, fractal dimension depends on material properties [27] and the mechanisms which lead to surface formation [28]. Therefore it is very important to understand how the growth parameters affect the fractal dimension and roughness of a surface. Obviously this knowledge will lead us to produce thin films or surfaces with desired properties.

The most part of our present knowledge about the processes leading to formation of fractal surfaces has been achieved from computer simulations. Simple computer methods for non-equilibrium growth and aggregation result in structures, which can be quantitatively described by fractal geometry. Aggregation processes are important phenomena that they have been subject of experimental, theoretical and simulation studies in many fields [29–31]. Diffusion limited aggregation (DLA) model [32] is one of the substantial models in theoretical and computational investigation of aggregation process. In this model, only a diffusion process describes the particles motions and the force between particles neglects. In DLA model particles are released on a surface one at a time, and after some random walks, they join to a growing aggregate (seed) of similar particles. In Multi-particle Diffusion Limited Aggregation model [29,33,34] a finite number of seeds exist instead of single seed of DLA model. In spite of simplicity, this model produces clusters showing complex behavior [35–38]. It offers a prototype of pattern formation in diffusive systems such as electrodeposition [39–41], dielectric breakdown [42], growth mechanism in thin films [43], and crystal morphology [44]. In addition, DLA model has also been generalized to simulate processes such as concentration [33], particle drift [45], surface tension [46], sticking probability [34,47–49], and heterogeneous surfaces [50].

In this work a multi particle DLA model is employed to simulate electrodeposition process. The significant future of this model is that, the radial motion with probability P competes with a random movement with probability $1-P$. This model gives more realistic description of growth in real materials due to existence of more than one microscopic growth mode. Our results show that the simulated thin films have anomalous behavior.

It is the first time that the morphology and kinetic roughening of electrodeposited thin films is studied using this model in 3D. On the other hand, the existing programs realizing multiparticle DLA model and fractal behavior often result in two dimensional figures. The program in this work can dynamically show the growth mechanism and evolution of electrodeposited thin films with fractal behavior in the form of 3D figures. Therefore, this simulation presents a much better description of fractal surfaces and their morphologies. In this study, the influence of different deposition conditions on morphology, roughness, scaling behavior and fractal dimension of electrodeposited thin films have been investigated. In spite of simplicity, these simulations can predict many features of the electrodeposited thin films.