ARTICLE IN PRESS

Physica A ▮ (▮▮▮▮) ▮▮▮–▮▮▮

Contents lists available at ScienceDirect

Physica A

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

Thin film growth models with long surface diffusion lengths

Tung B.T. To, Vitor B. de Sousa, Fábio D.A. Aarão Reis *

Instituto de Física, Universidade Federal Fluminense, Avenida Litorânea s/n, 24210-340 Niterói, RJ, Brazil

HIGHLIGHTS

- Limited mobility model reproduces surface morphology of collective adatom diffusion.
- Detachment probability from lateral neighbors has opposite effect on roughness.
- Effective mobility of adatom depends on its history in the film surface.

ARTICLE INFO

Article history:
Received 23 April 2018
Received in revised form 19 June 2018
Available online xxxx

Keywords:
Thin films
Growth models
Surface diffusion
Dynamic scaling

ABSTRACT

In limited mobility (LM) models of thin film deposition, the final position of each atom or molecule is chosen according to a set of stochastic rules before the incidence of another atom or molecule. Here we investigate the possibility of a LM model to reproduce features of a more realistic approach that represents the interplay of collective adatom diffusion and the external flux. In the LM model introduced here, each adatom may execute G hops to neighboring columns of the deposit, but a hop attempt from a site with n lateral neighbors has probability P^n, with $P < 1$. These rules resemble those of the Clarke–Vvedensky (CV) model without energy barriers at step edges, whose main parameters are the diffusion-to-deposition ratio R on terraces and the detachment probability ϵ per lateral neighbor. At short times, the roughness of the LM model can be written in terms of a scaling function of G and P and the growth exponent is consistent with the Villain-Lai-Das Sarma universality class. The evolution of the surface roughness and of the autocorrelation function of the CV model is reproduced with reasonable accuracy by the LM model with suitable choices of parameters. The increase of the parameters G and R of those models produces smoother film surfaces, while the increase of P and ϵ smoothen the terrace boundaries at short lengthscales. However, the detachment probabilities of the two models have very different effects on the surface roughness: in the LM model, for fixed G, the surface roughness increases as P increases; in the CV model, the surface smoothens as ϵ increases, for fixed R. This result is related to the non-Markovian nature of the LM model, since the diffusivity of an adatom depends on its history at the film surface and may be severely reduced after a detachment from a terrace step; instead, in a collective diffusion model, the detached adatom has the same mobility as a freshly deposited adatom in the same environment. This interpretation is supported by the correlation between the surface roughness and the average number of hops after the last detachment from lateral neighbors in the LM model. We conclude that, although a limited mobility model can reproduce morphological properties of a collective diffusion model, the role of apparently equivalent parameters may be very different, which have consequences for their physical interpretation.

© 2018 Elsevier B.V. All rights reserved.

* Corresponding author.
E-mail addresses: tungto@if.uff.br (T.B.T. To), vitorbento@id.uff.br (V.B. de Sousa), reis@if.uff.br (F.D.A. Aarão Reis).

https://doi.org/10.1016/j.physa.2018.07.024
0378-4371/© 2018 Elsevier B.V. All rights reserved.

Please cite this article in press as: T.B.T. To, et al., Thin film growth models with long surface diffusion lengths, Physica A (2018), https://doi.org/10.1016/j.physa.2018.07.024.

1. Introduction

Thin film growth models have been intensively studied in the last three decades due to a large number of applications and due to their fundamental interest in non-equilibrium statistical mechanics [1–4]. The most realistic models describe thermally activated microscopic processes such as diffusion, aggregation, desorption, and chemical reactions which simultaneously occur on the surface of the growing film; energy barriers for diffusion across step edges and various ranges of interactions between adatoms may be considered. The comparison between the parameters used in simulations of these models and those predicted by ab initio methods (e.g. density functional theory) may improve the description of a growth process and help the design of films with the desired properties [5]. Among the lattice models of thin film growth [5], one of the simplest examples is the Clarke–Vvedensky (CV) model [6], in which the diffusion coefficients have Arrhenius forms and the energy barriers represent interactions with the nearest neighbors in the lattice. Extensions of the original CV model have applications to molecular beam epitaxy of metals or semiconductors [1–5,7], vapor deposition of organic molecules, and deposition of colloidal particles [8–11].

Thin film growth may also be described with reasonable approximation by limited mobility models, in which the final aggregation position of each deposited atom or molecule is chosen according to a set of stochastic rules before the adsorption of another atom or molecule. Some well-known examples are ballistic deposition [12], the restricted solid-on-solid model [13], and the models for molecular beam epitaxy of Das Sarma and Tamborenea (DT) [14] and of Wolf and Villain (WV) [15]. Due to their simple growth rules, they are suitable for kinetic roughening studies, which require simulation of large systems and long times. Those studies provide estimates of quantities such as scaling exponents, height, and roughness distributions, which allow the connection between the lattice models and hydrodynamic growth equations that define universality classes [1,2]. However, an important question is whether limited mobility models with rules that mimic surface diffusion can be related to more realistic approaches such as the CV model.

A limited mobility model with this feature was studied in Ref. [16] and was subsequently termed lateral aggregation of diffusing particles (LADP) [17]. In that model, the incident atom can execute a maximal number of hops G on terraces and permanently aggregates if it has one or more lateral neighbors. For a suitable choice of parameters, its roughness scaling is the same as that of the CV model with irreversible attachment of adatoms to lateral neighbors; this is a case in which the CV dynamics do not obey detailed balance conditions. The DT, WV, and large curvature models with long diffusion lengths were also studied in several previous works [18–21], but no relation with models of collective adatom diffusion was proposed. An extension of the LADP model in which atoms with more than one neighbor can move was recently used to describe electrodeposition, in which porous films are formed [22].

In this work, we introduce a limited mobility model which is designed to represent mechanisms of surface diffusion similar to the CV model: each adatom can execute a maximum of G hops, detachment from lateral neighbors is allowed with probabilities depending on its current neighborhood, and solid-on-solid conditions are considered (i.e. the films are not porous). For simplicity, it is hereafter termed LM model. We determine the effects of its parameters on the scaling of the surface roughness and address the question of the equivalence with the original CV model. LM and CV models belong to the universality class of the nonlinear molecular beam epitaxy equation of Villain, Lai, and Das Sarma (VLDS) [23,24] and we show that it is possible to match the surface roughness and the autocorrelation function of the two models by a suitable choice of their parameters. However, significant differences are observed in the effects of the probabilities of adatoms detaching from lateral neighbors, which affect the physical interpretation of the LM model. These differences are discussed, with particular emphasis on the effective time of surface diffusion.

The rest of this paper is organized as follows. In Section 2, we present the models, the related growth equation, and the main quantities to be measured. In Section 3, we analyze the surface roughness in the LM model. In Section 4, we compare results of the LM model with those of the CV model. In Section 5, the effects of the detachment from lateral neighbors in the LM model are analyzed. In Section 6, we present our conclusions.

2. Basic concepts and definitions

2.1. Models

All models studied here are defined in a simple cubic lattice, with an initially flat substrate at $z = 0$. The edge of a site is taken as the length unit. The lateral size of the lattice is denoted as L and periodic boundary conditions are considered in the x and y directions. The set of adatoms with the same (x, y) position is a column of the deposit; the height variable $h(x, y)$ is the maximal height of an adatom in that column (or the number of atoms in the column).

2.1.1. CV model

Deposition occurs with a flux of F atoms per column per unit time, in the z direction towards the substrate. An incident atom is adsorbed at the top of a randomly chosen column. All adatoms at the top of the L^2 columns are mobile. The hopping rate of an adatom with no lateral neighbor is

$$D_0 = \nu \exp\left(-E_s/k_B T\right) \tag{1}$$

Please cite this article in press as: T.B.T. To, et al., Thin film growth models with long surface diffusion lengths, Physica A (2018), https://doi.org/10.1016/j.physa.2018.07.024.

Download English Version:

https://daneshyari.com/en/article/7374549

Download Persian Version:

https://daneshyari.com/article/7374549

Daneshyari.com