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New cellular automaton designed to simulate epitaxial films growth

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Abstract

In this paper, a simple $(2+1)$ solid-on-solid model of the epitaxial films growth based on random deposition followed by breaking particle–particle lateral bonds and particles surface diffusion is introduced. The influence of the critical number of the particle–particle lateral bonds z and the deposition rate on the surface roughness dynamics and possible surface morphology anisotropy is presented. The roughness exponent α and the growth exponent β are $(0.863, 0.357)$, $(0.215, 0.123)$, $(0.101, 0.0405)$ and $(0.0718, 0.0228)$ for $z = 1$, 2, 3 and 4, respectively.

Snapshots from simulations of the growth process are included.

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1. Introduction

Theoretical modelling of films epitaxial growth—which is the growth of an oriented single-crystal film of one material upon a single-crystal substrate of

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another [1] and the main microscopic process is particles deposition followed by their diffusion on the surface—may be grouped to continuum and discrete approaches [2].

The continuum approaches are based on the stochastic differential Langevin equations [3–6] which group models to the various classes of universality associated with the same set of critical exponents. In the discrete approach computational methods may be applied with *cellular automata* (CA) *technique* [9,10] among others. The latter bases usually on the Arrhenius-like kinetics [11,12] and requires knowing many parameters, for instance

- material and neighbourhood-dependent activation energies for different elementary processes,
- adatom/adatom, substrate-atom/substrate-atom and substrate-atom/adatom bonds strengths,
- vibration factors,
- substrate temperature,
- incoming particles flux, etc.

Usually, the values of these parameters are fitted to reproduce some experimentally measured particles and/or surface characteristics.

The title of Ref. [10] characterises the CA technique very well, as for CA, both discrete time and space are necessary. The model must also include the rule which tells how the states of lattice cells are subsequently updated. Usually, CA models for epitaxial growth simulations [13] rely on simple, or even toy, mechanical rules, e.g., random deposition followed by particles relaxation (see Ref. [2] for review). In the relaxation process particles often virtually move to the nearest-neighbourhood (NN) sites to check the accommodation conditions offered there and then choose the best one. Quite often, the subsequent particle arrives at the place of its first contact with surface only when previously deposited particle migration process has been completed. Such a situation corresponds to a very low flux of incoming particles and does not meet real conditions during molecular beam epitaxy experiments.

Here we would like to, present simple CA which loses both disadvantages of non-physical particles virtual movement to the NN sites and low particles flux, but still does not need material-dependent constants.

2. Model

The model presented here, is an extension to random deposition model (RDM) with additional particles relaxation. The solid-on-solid approximation is applied, so the film may be fully characterised by single-valued function $h(x, y, t)$ of the film height in planar coordinates ($1 \leqslant x \leqslant L, 1 \leqslant y \leqslant L$) in time t.

We start our simulation with perfectly flat substrate. Every τL^2 time steps a new jet of $\theta_{\text{dep}} L^2$ particles arrives. At each time step—between subsequent acts of the depositions—particles 'sitting' on the column top may diffuse on the surface. The