MONTE CARLO SIMULATION OF SIMPLE MODEL FOR THIN FILMS GROWN BY MOLECULAR BEAM EPITAXY

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1. Introduction

Crystal growth have been an area of great interest to the physics of condensed matter [1]. Technological applications make this one of the areas where computer simulation can help to understand microscopic processes and optimize laboratory time. There is no general rule for choosing the model used in a simulation [2]. In this work we have investigated the traditional Monte Carlo method [3] to study homoepitaxy of Si(001). This study includes re-evaporation and uses experimental embasement, obtained from literature, to apply in a future study of simulation of binary compound lattice-matched.

2. Theory

Monte Carlo simulation is a method for calculation of average values in a given equilibrium thermodynamical ensemble [3]. We consider a homoepitaxy, solid-on-solid (SOS) model, which does not allow formation of vacancies in an N x N square lattice substrate. Particles are randomly deposited in surface with a defined rate. In a Δt interval a certain number of particles are deposited and are allowed to attempt to hop to nearest neighbor sites or re-evaporate. The hopping rate is given by Equation 1.

$$R = R_0 e^{\frac{-nE}{K_B T}} \tag{1}$$

Where the attempt frequency is $R_0 \approx 10^{12} Hz$, n is the number of bonds, E is the "bond energy", T is the substrate temperature and K_B is the Boltzmann constant. The bond energy E, is in fact an effective energy, and do not have nothing to do with the chemical bond energy [3].

3. Results and Discussions

To test our model we simulated the growth of Si(001) homoepitaxy. There is no mismatch in the lattice. The binding energy were obtained from literature, and is 0.5 eV to vertical-binding and 1.0 eV to in-plane bindings [4]. We have simulated the growth for two parameters: the substrate temperature and the flux rate of impinging species. The flux rate were tested for 0.25, 0.50 e 1 Å/s. The substrate temperature was tested from 400 until 950 K.

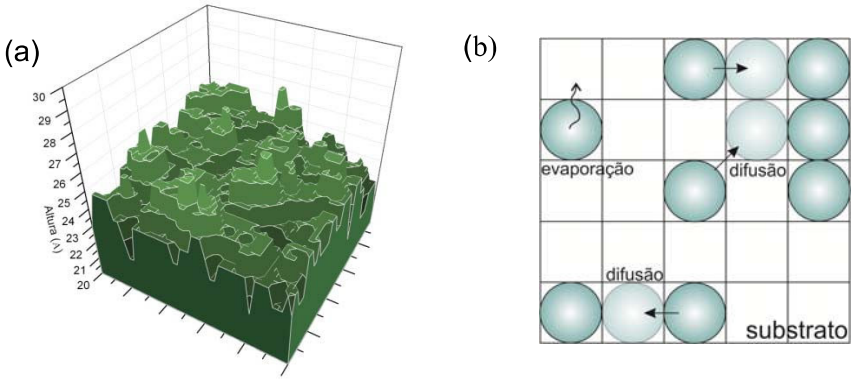

Fig. 1. **(a)** *Simulated surface of a thin film growth with 0.25 A/s and substrate temperature of 800 K.* **(b)** *Allowed growing processes in this simulation.*

4. References

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