

## SURFACE GROWTH MODELED BY AB-INITIO MONTE CARLO SIMULATION

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It is well known that certain materials show a granular structure in their surfaces, with hills of several heights and lateral extensions. Thermodynamic and kinetic determine how the film surface develops. Thermodynamic dictates the growing process, layer by layer, islanding or by a mixed mechanism. Kinetic plays an equally important role since island nucleation and growth is controlled by surface diffusion.

There are several ways of growing a surface. One of them is the ballistic-aggregation model [1] in which each particle added to the surface uses a linear trajectory with randomly selected direction to determine the final position. Another model is the Eden growth model [2] where particles are deposited on any point of the surface with equal probability. It is possible, as well, to describe the dynamic of growing surfaces by continual equations. Kardar, Parisi and Zhang (KPZ) [3] proposed a nonlinear differential equation which gives interfacial growth exponents consistent with numerical simulations of ballistic aggregation and Eden growth.

The main effort studying growing surfaces has been done experimentally [4,5]. We propose a simulation method to study the local behaviour of growing surfaces. This simulation is based on thermodynamic principles and uses two parameters: the energy increment  $E_0$ , obtained by having another atom in the position of a first neighbours, and the diffusion length average at the selected temperature.

It is possible to obtain the probability that an atom in a determined position can move to a close position. This is the elemental diffusion probability,  $p$ , and depends on the diffusion length average,  $\lambda$ . The bounding energy normalized to the thermal energy in a particular position is given by  $p^{\lambda/a} = 1/2$ , where  $a$  is the cell parameter. We define, as well,  $\mathbf{k}$  as a vector with the form  $\mathbf{k} = a(u_x, u_y, u_z)$ , where components  $u_i$  can value 1, 0, -1. The bonding energy normalized to the thermal energy is given by:

$$\varepsilon(\mathbf{r}) = \sum_{\mathbf{k}} \frac{E_0}{k_B T} \delta(\mathbf{r} + \mathbf{k}) \frac{|\mathbf{k}|}{a} \quad (1)$$

where

$$\delta(\mathbf{r} + \mathbf{k}) = \begin{cases} 1 & \text{if the position is occupied by an atom} \\ 0 & \text{if the position is not occupied by an atom} \end{cases}$$

An atom in a position  $\mathbf{r}$  has a transition probability to the  $\mathbf{r} + \mathbf{k}_0$  position given by a partition function:

$$P_{\mathbf{k}_0} = \frac{e^{-(\varepsilon(\mathbf{r} + \mathbf{k}_0) - \varepsilon(\mathbf{r}))}}{\sum_{\mathbf{k}} e^{-(\varepsilon(\mathbf{r} + \mathbf{k}) - \varepsilon(\mathbf{r}))}} \quad (2)$$

The algorithm used to simulate the theoretical behaviour is based on Monte Carlo method and it is divided on four steps:

1. An atom is deposited in a randomly selected position on the surface.
2. As a function of the probability of elemental diffusion,  $p$ , is randomly calculated if the

atom is going to diffuse:

- 2.1. The algorithm progress to the next step once the condition diffusion is fulfilled.
- 2.2. The atom is placed in the same position and the algorithm returns to step 1 when diffusion condition in not satisfied.
3. All the diffusion probabilities to first neighbours,  $P_k$ , are calculated and according to the obtained values the diffusion position is randomly selected. Here it is possible to apply Born-Von Karman boundary conditions if the atom leaves the simulation surface limits. In this case the atom enters again but, by the opposite limit of the surface.
4. The atom is displaced to the resultant position and the algorithm returns to step 2.

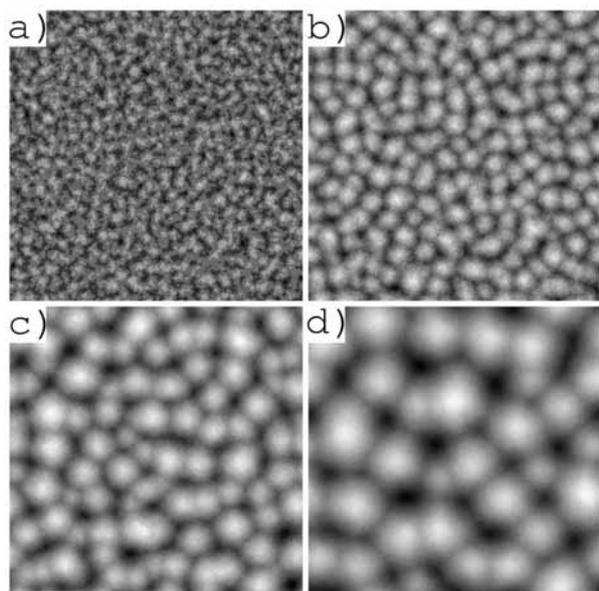
This simulation also takes into account the evaporation probability of an atom located on the surface. This evaporated atom has the same probability of being deposited again over the surface than the probability of finally being evaporated leaving a hollow in that position. If the evaporated atom is deposited over the surface, it starts again the diffusion process.

Fig.1 shows the evolution of the growing surface simulation. As thickness increases it can be observed that the density of mounds decreases, raising its size. This appearance is very similar to the experimental ones, presented on the literature [5]. As the average surface thickness increases, the maximum value of the power spectrum moves to lower frequencies (Fig.2). It can be also observed that the Fourier transform maximum value increases in amplitude. This maximum value is related with the average size of surface mounds and therefore with the bonding energy. These results prove that the model is good enough to explain the local behaviour of growing surfaces.

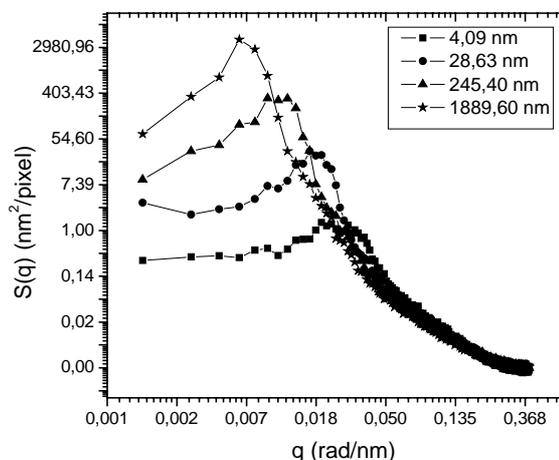
## References

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## Figures



**Fig.1.** Simulation obtained figures with bonding energy  $\varepsilon=E/kT=0.5$  and diffusion length average 40.9 nm,  $512 \times 512$  pixels<sup>2</sup> of resolution and  $125 \times 125$  nm<sup>2</sup> size. The growing film thickness is: a) 4.09 nm.



**Fig.2.** Power spectrum vs thickness. Growing parameters:  $\varepsilon=E/kT=0.5$  and diffusion length average 40.9 nm,  $512 \times 512$  pixels<sup>2</sup> of resolution and  $125 \times 125$  nm<sup>2</sup> size

size. The growing film thickness is: a) 4.09 nm, b) 28.63 nm, c) 245.40 nm and d) 1889.60 nm.