Model of diffusion packing colloidal particles

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Abstract. This paper describes a computer model for the formation of thin films by sedimentation of colloidal particles with allowance for surface diffusion with various methods of self-organization. The process of organizing such films similar to the free fall of identical balls that form an organized structure. Understanding the self-assembly mechanisms of nanoparticles is an important step in the direction of creating new materials with regard to optical and electrical properties.

1. Introduction
Even at the early stage of thin-film research, it soon became clear that it was necessary to understand the mechanisms that control and determine the growth of thin films in order to achieve good control over these new materials [1]. Hence, the great efforts of the scientific community to characterize optimize and understand the growth of thin films [2-8]. In connection with the need for a high degree of control above the properties of the films was proposed a computer model that is a stochastic cellular automaton. This model is of interest due to simple deterministic rules that allow modeling not only the processes of deposition, but also the diffusion of deposited particles on the surface.

Figure 1. Particles deposited according to the proposed spatial lattices.
This paper considered the processes of deposition of thin films on a substrate of the same material, forming a crystalline structure. The homo-epitaxial growth of thin films is interesting because the crystal structure doesn't change with the growth of the film; therefore, this model's particles can occupy only ideal crystallographic positions [9-10].

2. The types of spatial organization of particles
In this model, seven possible spatial lattices were considered: three of which have a rectangular grid at the base and four that have a triangular grid at the base. In addition, these spatial lattices divides by according to the type of fixing new particles relative to the previous monolayer.

In the figures 1.a, 1.b, and 1.c inside each monolayer, the centre of each particle fixes at the nodes of a uniform rectangular grid, in the structures 1.d, 1.e, 1.f, and 1.g – uniform triangular grid.

When placing particles into crystal lattices 1.a and 1.d coordinates of the centre of each particle inside the monolayer repeat the coordinates of the centres of the previous particles, i.e. particles in each layer are directly over each other, thus it argues that their coordinates repeats with a period equals one monolayer.

In the case of placement type 1.b and 1.e, the coordinates of the centre of each particle inside the monolayer with each subsequent layer shifts by half the grid division in the direction of one of the axes. So each particle is held by two particles of the previous layer (for all but the first) and the repetition period of coordinates particles is two monolayers.

The spatial grid 1.c is a structure of ordered particles, where each particle places over the four particles of the previous layer, overlapping the gap between them, i.e. its centre is over the centre of the rectangular grid cell of the previous monolayer. The repetition period of the particle coordinates is also two monolayers.

Cases 1.f and 1.g also represent the structure of ordered particles, where each particle places over the centre of the grid cell of the previous monolayer, overlapping the gap between them. However, in connection with the binding of the location of particles inside each monolayer to the nodes of a uniform triangular grid, the number of neighbouring particles of the previous layer is three. The repetition periods of the position of the layers in the structures are two monolayers in the case of 1.f and three monolayers in the case of 1.g.

3. The deposition model of particles
All new particles are identical and their places of deposition are random, and more than one particle doesn't deposit in one node of the spatial grid at one simulation step. The number of particles that hit the surface at one simulation step determines the deposition rate of particles. Upon completion of the deposition of new particles for each of the points of the surface in which the new particle is located and its nearest neighboring points, the probabilities of diffusion of the particle are calculated [11].

Figure 2. The two-dimensional case of the first-order Moore region for: a) rectangular grid; b) triangular grid
Figure 3. Simulated colloidal structures. The deposition time is 50 simulation steps. The deposition rate is 0.1 monolayer per simulation step. The average film thickness is 5 monolayers. Spatial lattice: a) Figure 1.a; b) Figure 1.d; c) Figure 1.b; d) Figure 1.e; e) Figure 1.c; f) Figure 1.f; g) Figure 1.g.
The nearest neighbouring particles are particles whose centres are in the Moore region of the first order [12]. A spatial grid node belongs to the first-order Moore region of the node in question if it's locates in the same cell as this node (figure 2).

After that, in accordance with the calculated probabilities, the particle diffuses to the corresponding point on the surface.

4. Results and conclusions
In the consequence of numerical calculations of the obtained surface of colloidal structures shows in figure 3.

Figure 3.a shows a structure based on a spatial grid of type 1.a. This structure has the largest through gaps between the particles (among presented), the maximum fillable volume and the large value of the standard deviation of the film thickness from the average value (defined as roughness).

Figure 3.b, a structure based on a spatial grid of type 1.d. The through gaps between the particles reduces about four times in relation to the structure 1.a, due to which the filling volume decreased by 14%, the diameter of the islands increased.

Figure 3.c and 3.d, at the structures, the size of the gaps decreases about five times and the filling volume decreases by another 14% in relation to the structure 3.a and 3.b respectively. The structure of the film is more like the fibres, but not the islands. The surface is smoothed by increasing the surface tension.

The fractal dimension of the surface of the structures 3.e, 3.f and 3.g tends to two. Particles of thin film 3.g packs as closely as possible. In structures of types 1.c and 1.g with a thickness of more than three monolayers, through gaps are absent (Figure 3.g and 3.e).

Thus, we can directly control the optical properties and electrical conductivity of thin films due to the possibility of choosing the type packing of particles in colloidal structures.

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