Mathematical modeling of the structure and optical properties of the fractal island metal nanofilm

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Abstract. The article discusses the experimental results of the fractal metallic island nanofilms elaboration and their modeling in the DLA approximation. There is also presented the simulation of their optical properties using the Monte Carlo method and the scattering intensity, based on the fractal characteristics.

1. Introduction

Today, island nanofilms made of gold and silver and their mixtures take a wide range of applications in various applications of nano and microelectronics, which is associated with the uniqueness of their structure and the electrical and optical properties shown by them.

Thus, the optical properties of nanofilms on substrates of various nature are of scientific interest from the point of view of modifying the properties of the media, in essence creating new materials based on well-known ones. It is obvious that the optical properties significantly depend on the structure of the nanofilm. In this connection, there is a need for mathematical models describing the structure and properties of island Ag, Au, Ag / Au films, which, in the first approximation, will allow us to calibrate the proposed experimental method for their preparation.

2. The results of experiments on the noble metal island films preparation

There are a large number of methods and processes for producing thin films - from rolling to the deposition of material on a substrate atom by atom. Most commonly used precipitation methods. For the formation of metallic island films by laser deposition, a prepared colloidal solution of gold and silver nanoparticles was deposited on a capillary substrate with a diameter of 50 μm (ground glass K-8), preheated to 60 ° C, in a thin layer with a height not exceeding 1 mm. After laser irradiation and formation of clusters on the surface of the substrates, they were studied using the Integra-Aura probe nano-laboratory.

In all cases, in the process of deposition, cluster structures of dendrite type are formed on the surface of the glass substrate. Moreover, in the structure of clusters, individual particles with sizes of 30–100 nm are well distinguished, the sizes of which, however, exceed the diameters of the particles in the original colloid, which makes it possible to speak of the aggregation of particles before sedimentation. [1]

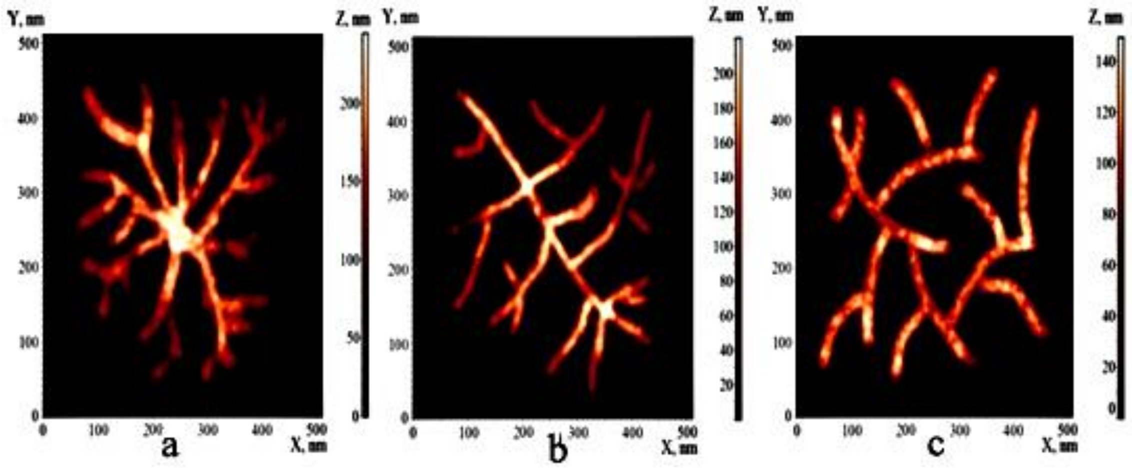

Figure 1. AFM images of the deposited cluster structures Ag (a), Au (b), Ag / Au (c).

3. Island film structure model

The DLA model was chosen to describe the formation of island film aggregates for several reasons: the results of experimental studies show that thermal diffusion takes place, which is quite well modeled in the DLA approximation, and the elements of the experimental film are visually similar to the fractal clusters obtained by the DLA algorithm [3] with inherent fractal properties. [2]

The algorithm consists of steps:

1) on a square two-dimensional lattice, a germ structure is specified;
2) away from the cluster (from the embryo) a new particle is born;
3) a new particle wanders randomly;
4) if a particle comes to a busy cell, then it sticks with a given probability;
5) if the particle moves far enough away from the cluster, it is destroyed;
6) repeat from step 3 until the particle sticks or dies, after which a new particle is launched.

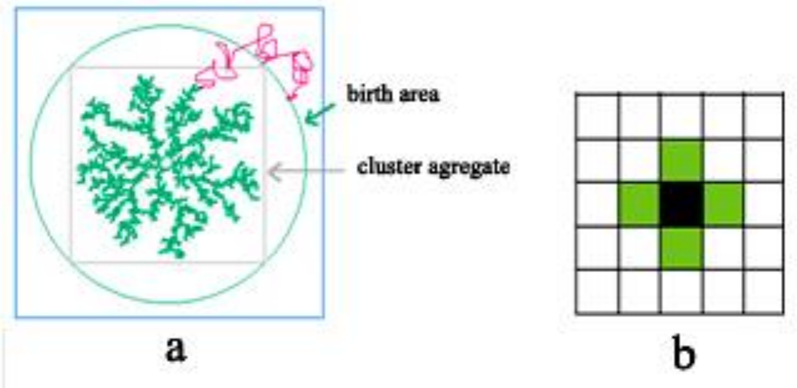

Figure 2. Island model: DLA scheme (a), von Neumann neighborhood (b).

In the simulation, the initial concentration and the probability of sticking of particles and aggregation centers were varied within a two-dimensional von Neumann neighborhood of order 1. To simulate different types of hot-film films, various configurations of the initial conditions for the DLA method were considered depending on the seed particles: with one seed particle (Fig. 3) and several seed particles (Fig. 4). Since there is no interaction between particles in the model, only the interaction of a free particle and a fixed cluster is considered. Growth centers of aggregates are thrown into space randomly.

The effect of the sticking probability on the shape of the film island can be estimated from Figure 2. As the sticking probability decreases, the generated fractal becomes almost evenly distributed at the edges. [4]

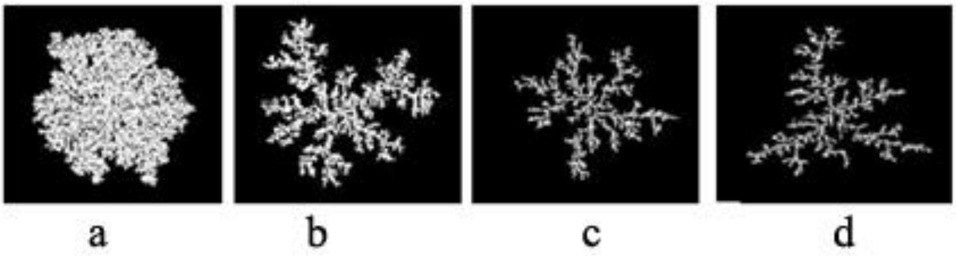

Figure 3. Model images of fractal structures of a film island with a sticking probability: a) 0.01 b) 0.1 c) 0.5 g) 1.

The case of the growth of aggregates from an initially homogeneous system (Fig. 4) in which, most likely, we should expect the simultaneous appearance of several clusters and their growth due to the absorption of small particles, as well as sticking to each other, was also considered.

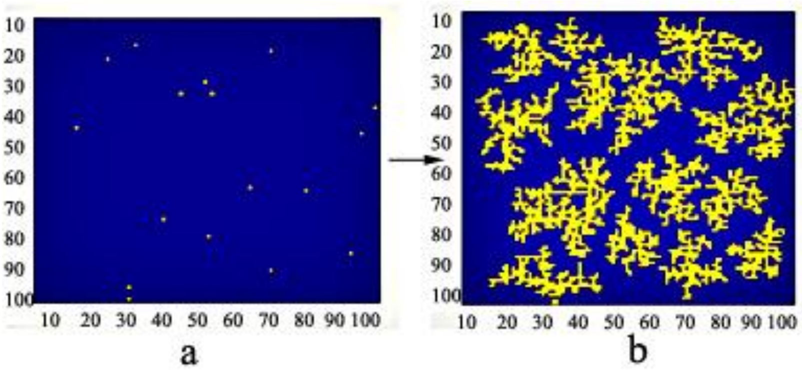

Figure 4. Film with several centers of aggregation. a) the initial random distribution of nuclei with a sticking probability of 0.5 (b) formed islands.

For the modeled structures, the fractal dimension was calculated, which was calculated as d = log (n) / log (r), where n is the number of particles that make up the fractal structure, r is its radius. When varying the probability of sticking from 0.01 to 1, the fractal dimension varied in the interval from 1.66 to 2.06 [5]. For example, for individual islands, the radius was 83.8276 rel. units, and the fractal dimension is 1.8286. The calculation of the characteristics mentioned above allows, in the first approximation, to estimate the size of the islands of the nanofilm, going from relative to absolute units by specifying the characteristic size of the particle. So for an island with a radius of 83.8276 rel. units specifying a particle size of 10 nm, one can estimate the absolute radius as 838.267 nm., which coincides qualitatively with the results of the Integra-Aura probe nano-laboratory. [6]

4. Model of optical properties of an island film in the Monte Carlo approximation

Of particular interest is the description of the modeling of the optical properties of the obtained island films.

The heuristic nature of the theory of the transfer of light radiation allows the use of Monte Carlo methods to simulate the transfer of photons through absorbing and scattering media due to its flexibility and simplicity for arbitrary geometries with complex boundary conditions. [7]

In the proposed model, the local photon migration rules are determined by random walks, which are represented as probability distributions, which describe the pitch of the photon in the medium and angles to which the scattering trajectory deviates. Thus, the basic procedure of the Monte Carlo method is as follows: a photon is triggered and then the trajectory of its movement is tracked and analyzed. The model operates with relative units, where the possible pitch of the photon corresponds to the reciprocal of the adsorption coefficient: ds = 1 / μ, and the step length is dr = ds * rand, where rand is a uniformly distributed random number. Then the actual length (probability) is calculated as drf = exp (-μ * dr), and the deviation angle corresponds to Θ = (4π * rand - 2π).

Figure 5 shows the trajectory of the photon with a relative coefficient adsorption 0.1 per 100 random walk steps.

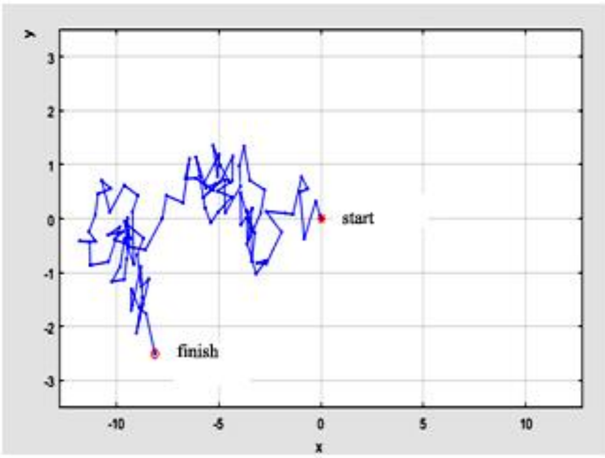

Figure 5. The trajectory of the photon, the adsorption coefficient of 0.1, 100 steps

The case of taking into account the substrate was also considered when the adsorption coefficients of the substrate and the island were specified, and the photon was moving taking into account the fractal island formed (Fig. 6).

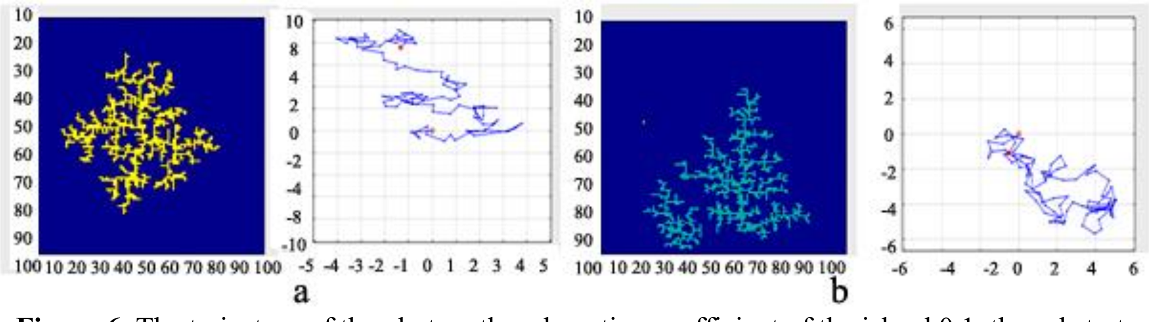

Figure 6. The trajectory of the photon, the adsorption coefficient of the island 0.1, the substrate 0.2, 100 steps (a) one island (b) two islands.

5. Model describing the intensity of radiation scattering on a fractal cluster

Based on the fractal nature of an island of nanofilms, it is also possible to simulate its optical properties. For example, the intensity of radiation scattering on a fractal is proportional to the Fourier component of the material density in it: $S(k) \sim k^{-D}$, where S is the intensity of the scattered light, k is the photon wave vector ($k = 2\pi / \lambda$, λ is the wavelength) , D is the fractal dimension of the island of the nanofilm [8] (Fig. 7).

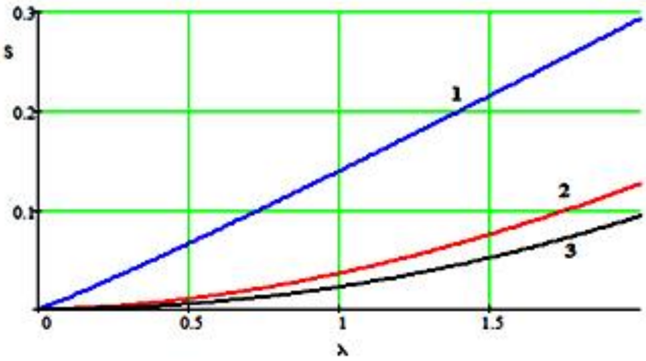

Figure 7. Scattering intensity from wavelength rel. Units: 1: D = 1.07, 2: D = 1.8, 3: D = 2.06

6. Conclusion

The character of the obtained model dependences corresponds to the theoretical and experimental data [5], which allows in the first approximation to apply this approach to the study of the structure and optical properties of metallic island nanofilms.

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