Structural and scattering characteristics model of a fractal nanoclustered island Ag-Au films

D.N. Bukharov, O.A. Novikova, S. P. Eyoum Essaka., S.M. Arakelian
Vladimir State University, 87 Gorky str., Vladimir, 600000, Russia
buharovdn@gmail.com

Abstract. Samples of Ag/Au nanocluster/island fractal nanofilms obtained by thermal diffusion deposition from a colloidal solution are presented. Modeling and evaluation of the features of their structure in the approximation of diffusion-limited aggregation are carried out. The evaluation of the scattering characteristics of the study on the model samples in the framework of the Fischer-Burford relation is made.

1. Introduction
Today, nanocluster/island films of noble metals are widely used in various applications of nano- and microelectronics, which I associate with their electrophysical and optical properties due to the uniqueness of their structure. For a number of years, the team of authors of this article has been conducting experimental studies on the preparation of samples of Ag/Au nanofilms by laser methods, which allow the formation of the required properties.

2. Description of experimental studies on obtaining Ag/Au nanocluster films
The original bimetallic Ag/Au films were obtained by laser thermal diffusion metal deposition from colloidal solutions of nanoparticles [1], which made it possible to obtain ensembles of nanoclusters on the substrate surface that form a nanocluster/island nanofilm. Images of the obtained samples were studied using the Integra-Aura probe nanolaboratory and MATLAB tools. As a result, it was found that the films have a fractal structure. For example, in the process of deposition on the surface of a glass substrate, cluster structures of the dendrite type were formed (Fig. 1) [1]
3. Model of the structure and scattering characteristics

Due to the dendritic structure, as well as the thermal diffusion nature of deposition, nanoclusters / film cuttings were modeled within the framework of diffusion limited aggregation (DLA) [2]. The process of structure formation was realized by the cellular automaton method with the von Neumann neighborhood, when the movement was made in 4 directions and the state of 4 neighboring cells, relative to the current one, was analyzed [4].

The algorithm consists of steps (Fig. 2):
1) a nucleus structure is set on a square two-dimensional lattice;
2) far from the cluster (from the nucleus), a new particle is generated in the nucleation region of the computational domain Rp;
3) the new particle wanders randomly;
4) if a particle approaches an occupied cell, then it sticks with a given probability;
5) if the particle moves far enough from the cluster, it is destroyed outside the outer sphere Re;
6) repeat, starting from step 3 until the particle sticks with a given probability, after which a new particle is launched [6].

For the obtained model samples, the values of fractal dimensions were calculated by the method of concentric circles in accordance with the ratio \( d = \log (n) / \log (r) \), where \( n \) is the number of fractal points enclosed in a circle of size \( r \) [7].

In fig. 3 shows the images of the islands for the computational area of 330 * 330 rel. Units, \( R_p = 100 \) rel. Units; \( R_e = 150 \) relative units, with varying the sticking probability \( \alpha_c \), after a time equal to \( t = 105 \) relative units, for which the fractal dimension \( D \), radius \( R \) and the number of particles \( N_c \) of which they
consisted were estimated. By comparing the model images, one can estimate the influence of the sticking probability on the shape and fractal dimension of the film islands.

The performed computational experiments and their statistical processing showed that the diffusion-limited aggregation model allows one to obtain fractal clusters with dimension $D$ in the range from 1.63 to $2.02 \pm 0.03$ when the probability of Sc adhesion changes from 1 to 0.01 on a two-dimensional lattice (Fig. 3) and is well described by the dependence: $-0.067\ln(Sc) + 1.63$. [3]

Analyzing the dynamics of the cluster formation process, it can be established that at the beginning of the process a large number of small clusters were formed. Later they were combined into larger units. Thus, over time, the number of clusters in the volume decreased and their sizes increased.

So in fig. 2 g, 3 nuclei were originally assigned, two of which (the second and the third) united into one cluster, with a sufficiently high value of the fractal dimension. In Fig. 2e, four embryos are combined into a single cluster. Thus, at a low value of the adhesion probability, before the moment of attachment to the cluster, the particles passed further along the computational domain, in contrast to the case of a high value of the adhesion probability.

At a high value of the sticking probability, fractal clusters will have a rather loose structure and a strongly indented boundary (Fig. 2 b, c, d) with a lower value of the fractal dimension, in comparison with clusters obtained at low values of the sticking probability, which have a well-filled structure and a sufficiently smooth boundaries, and as a consequence, a large fractal dimension (Fig. 2 a, e). Thus, the adhesion probability parameter, which takes into account the intensity of thermal diffusion in the simulated system, significantly affects the shape of the nanofilm islands: at its low value, islands with high occupancy are generated, and at a high value, with low degrees of filling.

![Fig.3](image-url) Model images of Ag / Au nanofilm islands: $D = 2.02$, $Nc = 9007$, $Sc = 0.01$, $R = 94.475$ (a), $D = 1.7845$, $Nc = 2705$, $Sc = 0.5$, $R = 83.815$ (b), $D = 1.7839$, $Nc = 2679$, $Sc = 0.6$, $R = 83.4865$ (c) $D = 1.8137$, $Nc = 3052$, $Sc = 0.3$, $R = 83.4086$ (d), $D = 1.9412$, $Nc = 5391$, $Sc = 0.03$, $R = 83.6301$ (e).

The scattering characteristics were estimated as an averaged function of the scattering intensity $I(q)$ depending on the scattering wave vector $q = 4\pi\sin(\theta)/\lambda$, where $\theta$ is the scattering angle, $n$ is the refractive index of the medium, $\lambda$ is the wavelength of the incident radiation. In our experiments, we used a micrometer source $qR_0 \ll 1$, where $R_0$ is the radius of gyration of the initial cluster; therefore, the Fischer-Burford relation is applicable for the estimation

$$I(q) = I(0)/(1 + 2(qR_G)^2/3D)^{D/2},$$

where $I(0)$ is proportional to the mass dimension of the cluster $M_W \sim R_G^D$, where $R_G = n_c^{1/D}$ is the radius of gyration, $n_c$ is the number of particles in the cluster [5].
Fig. 4 shows the dependence of the intensity on the wave vector for the samples from Fig. 3a, b. for the case of micrometer radiation. The estimation results show its increase with decreasing fractal dimension. This behavior is explainable due to the complication of the film relief, the appearance of many peaks, cones, and complex surfaces on which scattering occurs.

![Fig. 4. Dependence of the scattering intensity on the wave vector.](image)

4. Conclusion
Thus, the proposed models allow, in the first approximation, at a qualitative level to evaluate the results of the experimental studies.

Acknowledgments
The reported study was funded by RFBR, project number 20-02-00515.

References
[1] Antipov A A, Arakelian S M, et al 2014 Optics and spectroscopy 116(2) 349-352.
[2] Batyukov A M. 2014 Computer tools in education 3 3-8.
[3] Belko A V, Nikitin A V, Skaskevich A A, Bachurina A Yu, Sarosek S I. 2012 Bulletin of Yanka Kupala State University of Grodno. Series 2. Mathematics. Physics. Informatics, computer engineering and management 2 95-104.
[4] Lobanov A I 2010 Computer Research and Modeling 2(3) 273-293.
[5] Ferri F, D’Angelo A, Lee M, Lotti A, Pigazzini M C, Singh K, Cerbino R 2011 Eur. Phys. J. Special Topics 199 139–148.
[6] Mroczka J, Woźniak M, Onofri F R A 2012 Metrol. Meas. Syst. XIX (3) 459-470.
[7] Yanguang C, Yihan W, Xijing L 2019 Chaos, Solitons & Fractals 126(C) 122-134.