Electrical conductivity of the thin films grown by random shaped clusters

Zh. Ebrahiminejad, S. Farhad Masoudi, and H. hamzehpour

***Abstract*—** In present work, using Monte Carlo technique, a rough and porous thin film recently simulated by deposition of randomly shaped clusters with different sizes on an initially flat substrate. The scaling exponents are calculated and found to agree with the ballistic deposition model. Then, effect of cluster size on the scaling exponents is studied. Moreover, the bulk porosity and its dependence on time and cluster size are also surveyed. As the behavior of film's conductivity affects by its morphology, in continue, the electrical conductivity of these porous solid films which grown by random shapes and sizes clusters is investigated. The conductivity is computed as a function of several relevant parameters. Based on our results, the frequency-dependent effective conductivity is a decreasing function of the cluster's sizes, such as porosity. The effective conductivity σ_e and dc conductivity depends on the frequency and the clusters sizes through a power law, respectively.

***Keywords*—** Electrical conductivity, Porosity, Random shaped clusters, Rough solids

I. INTRODUCTION

FOR few decades the conduction analysis have drawn attention to experimental and theoretical works [1-3]. One of the most interesting behaviors of ac and dc conduction is observed in disordered/rough solids in experimental results, modeling, and computer simulations. It is well established that ac conduction is dependent on properties of disordered/rough thin solid films. Therefore, because of practical applications of thin films in electronic devices, the surface physics become one of the most interesting branches of condensed matter research [4-7]. There are various theoretical methods to grow the thin films with different statistical properties and dynamic progresses. These methodes used frequently for describing the surface growth and kinetic roughening of thin films [8]. In recent work, a rough and porous thin film recently simulated by deposition of randomly shaped clusters with different sizes on an initially flat substrate using Monte Carlo (MC) technique. In analogy with the ballistic deposition process, our approach results in aggregation of clusters with a porous bulk and a rough surface that obeys the Family-Vicsek dynamic scaling. The scaling exponents are calculated and found to agree with the ballistic deposition model. Moreover, the bulk porosity and its dependence on time and cluster size are also investigated. We have also studied the influence of the cluster size on the scaling exponents and the stationary porosity [9].

in the present work we are interested in calculation of frequency-dependent conductivity in bulk and porous thin films which are grown by cluster deposition. As the thin films are grown by deposition of identical or different shapes clusters, here, we consider the different size's clusters to investigate the effect of the size and shapes of clusters on conductance. Also, for calculating of conduction the macroscopic model is used, which is derived from Maxwell's equations. It is assumed that the thin solid film has free charge carriers that are characterized by a local conductivity as well as bound charges presented by the spatially constant dielectric constant [10,11].

The article is organized as follows. In Sec. II, we give a brief description of the macroscopic model and its discretization. Computer simulations and interpreting of results are presented and discussed in Sec. III. Conclusions and final remarks are in Sec. IV.

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II. THE CONDUCTION FORMALISM

In this section, we provide the mathematical foundations and relations related to the dc and ac conduction in a rough porous surface. The free charge carriers of solid surface are characterized by spatially varying and frequency-independent local conductivity g(**r**). The bound charges are denoted by a fixed dielectric constant ε_{∞}. The constitutive equations are as follows:

$$\mathbf{D}(\mathbf{r},t) = -\varepsilon_{\infty}\nabla\phi(\mathbf{r},t), \quad (1)$$

$$\mathbf{J}(\mathbf{r},t) = -g(\mathbf{r})\,\nabla\phi(\mathbf{r},t), \quad (2)$$

where, **D, J** and ϕ denote the displacement vector, the free charge carrier current density and the electrostatic potential, respectively. Combining these equations with the Gauss' law

$$\nabla.\mathbf{D}(\mathbf{r},t) = \rho(\mathbf{r},t), \quad (3)$$

where ρ is the free charge carrier density, and continuity equation

$$\frac{\partial}{\partial t}\rho(\mathbf{r},t) + \nabla.\mathbf{J}(\mathbf{r},t) = 0, \quad (4)$$

we retrive the following relation:

$$\nabla.\left[\varepsilon_{\infty}\frac{\partial}{\partial t}\phi(\mathbf{r},t) + g(\mathbf{r},t)\nabla\phi(\mathbf{r},t)\right] = 0. \quad (5)$$

Considering space time dependency, e^{iwt}, for all quantities in a periodically varying field and introducing the Laplace frequency as $s = iw\varepsilon_{\infty}$, we obtain:

$$\nabla.\left([s+g(r,t)\nabla\phi(r,t)]\right)=0, \quad (6)$$

Discretizing equation (6), we end up with a electrical equivalent circuit (EEC). The resistors in the EEC are further proportional to the inverse free charge conductivity $g^{-1}(r)$ which correspond to the free charge currents. Spatial variation of the resistors represents the surface conductivity. All the capacitors in the EEC are equal and are proportional to the fixed dielectric constant. A potential difference is then applied to two opposing faces of the circuit and the admittance between these faces is denoted by y=k(s+g) where k is a constant. In EEC is defined on a lattice in which each link is a parallel resistor and a capacitor. The electrostatic potentials at the nodes can further be obtained by solving Kirchhoff's equations. Furtheremore, the resistor's current is denoted by I_R , the free charge current is given by **J**= I_R/a^{D-1} , where *a* is the lattice constant, and D is the spatial dimensional. The potential drop across a link is denotes by $\Delta\phi$. We therfore have $I_R = kg\Delta\phi$ and $J = g\Delta\phi/a$. Eventually, the parameter k is defined as $k=a^{D-2}$.

The admittance on each link is further given by

$$y= a^{D-2} (s+g). \quad (7)$$

Two opposing faces of the surface are considered as electrode and the current between them is calculated as

$$I(s) = Y(s)\Delta\phi(s), \quad (8)$$

There are (N-1) series of parallel RC elements with the same total current I(s) between the electrodes. The overall frequency- dependent conductivity of the parallel RC elements are therefore given by,

$$\sigma_e(s) = Y(s)L^{2-D} - s, \quad (9)$$

All of the resistors and all capacitors of the EEC are considered to be equal. For the linear dimension of the circuit with L in D dimensions, the effective conductivity of networks with equal linear sizes reads

$$\sigma_e(s) = \frac{h}{L^{D-1}}Y(s) - s, \quad (10)$$

By using the finite volume method and the divergence theorem, we integrate Eq. (6) over the system's volume and end up with

$$\int_V \nabla.[(s+g(r))\nabla\varphi(r,s)]dv = \int_{\partial r}(s+g(r))\nabla\varphi(r,s).dA = 0. \quad (11)$$

Here, ∂v and dA are system's surface and surface elements, respectively. One can check that the net current passing through each network block is zero (second integral in Eq. (12)). In the followin, the net flux through a square grid block is calculated based on the sum of the integrals over its four faces:

$$\int_{\partial v} J.\,dA \cong \sum_{k=1}^{4} J_k A_k = 0, \quad (12)$$

where, A_k is the surface area through which the current $J_k$flows. For each block centered at (i,j) the Eq. (12) is discretized as:

$$J_{i+1/2,j} + J_{i-1/2,j} + J_{i,j+1/2} + J_{i,j-1/2} = 0, \quad (13)$$

where each term in Eq. (13) is related to a unit cell size and the conductivity between two neighboring blocks. For example, the conductivity between the blocks centered in (i,j) and (i,j-1) is proportional to

$$g_{i,j-1} = \frac{2g_{i,j}g_{i,j-1}}{g_{i,j}g_{i,j-1}}, \quad (14)$$

Other terms of Eq. (13) have the same expression. The matrix representation of the above linear equations are expressed as

$$A.\varphi = B, \quad (15)$$

where, φ and **A** are sparse matrices which reperesent the electrostatic potential, respectively and **B** is related to a driving force ΔV. Equation (15) is solved by the biconjugate-gradient method [12].

III. RESULTS

In our simulations, the periodic boundary condition is considered in both directions and between the top of the surface and the substrate, a constant potential ΔV in vertical direction is also applied to the surface. The distributions of electric potential in films for different sizes of the substrate and different frequencies are shown in Fig. 1.

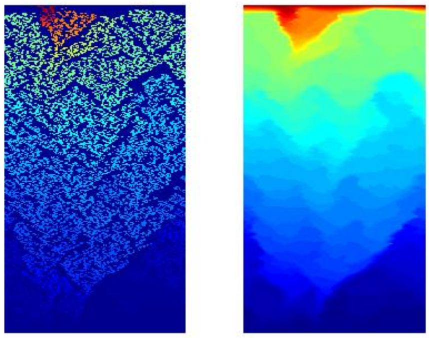

Fig.1. The distributions of electric potential in films for N=4a and L=256a. s=0 (left) and s= 2.3×10^{-4} (right).

The effective conductivity is calculated as a function of cluster's sizes, time, frequency and time evolution of the porosity. Fig. 2 shows the $\sigma_e(s,t)$ as a function of time. There are two interesting points in all cases of Fig. 2. The first is that, in all cases, dependence on cluster's sizes and frequency, σ_e saturates to specific values. And as the second point, it can be ssen that the effective conductivity of rough porous strctures has the highest value for the smallest cluster's sizes. The reason of the latest point is that the smaller clusters have smaller porosities so it has no main contribution in the net conductivity. In ref [9], the morphology of surafce has been well studied, the steady state, the porosity of surface reaches to a saturation value for each cluster'sizes. Then the saturation of effective conductivity ocuures because the saturation of film's porosity. It is worthable to note that in Fig. 2, the value of frequency and cluster'sizes have a behaviour with time saturation of σ_e in all cases. As the frequency (s) increase, the conductivity increase too, and imact of film's morphology reduces with increasing the frequency [10, 11].

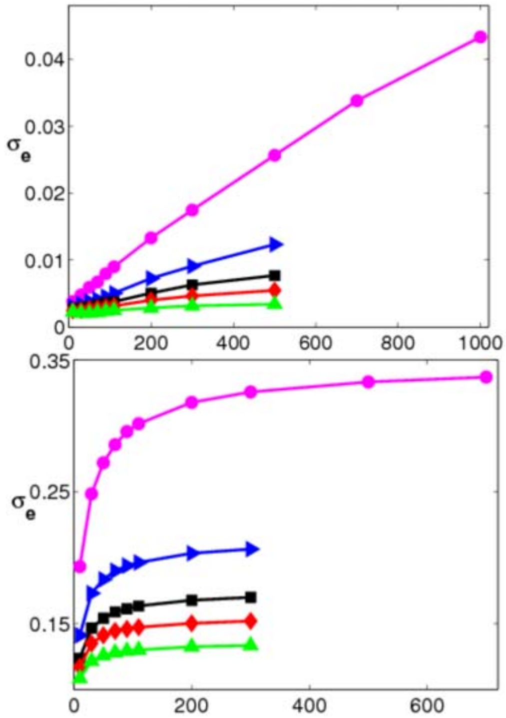

Fig. 2. The effective conductivity σ_e as a function of time t for L=512a and frequencies, s=0(Top figure), 0.01(bottom figure). The results are for the particles sizes 2a, 4a, 6a, 8a, and 12a (from top to below).

As the clusters have the random shapes and sizes, the growing surfaces are porous [9]. Fig.3, shows a part of rough porous thin films which are produced by random shaped clusters.

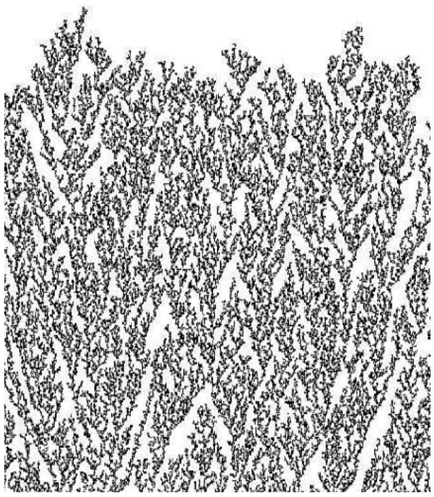

Fig. 3. A piece of porous films that are grown by deposition of random shapes and sizes clusters.

The results of Fig. 2 shows that the σ_0 depends on stationary porosity value. So this dependency presents in Fig. 4. This dependency is linear and for the range of cluster's size which the cluster size increase with increasing the porosity, the data approximated by the following equation:

$$\sigma_0 \approx -0.23\varphi_s + 0.17 \quad , \quad (16)$$

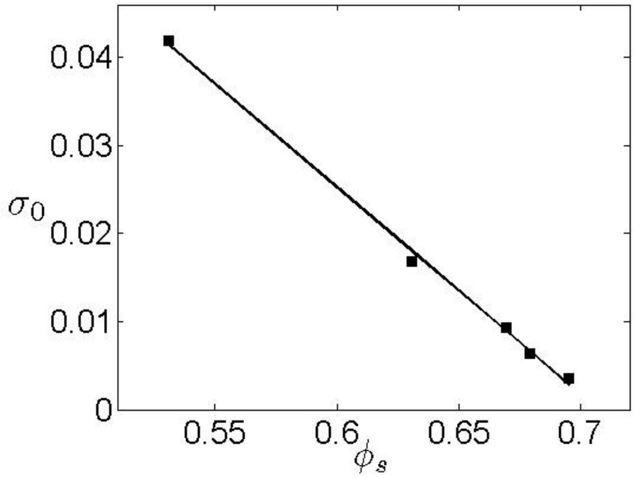

Fig. 4. The dependence of the dc conductivity σ_0 on the saturated porosity ϕ_s.

IV. Conclusion

In this paper, we studied the frequency-dependent effective conductivity of porous thin films which these films are grown by different shapes and sizes clusters and its dependence to several properties. Our findings showed that the effective conductivity is related to the film's morphology. The frequency-dependent effective conductivity σ_e, is a decreasing function of the deposited cluster's sizes, as well as the porosity. Therefore, the σ_e, decreases with increasing the clusters sizes. The dc conductivity σ_0, as a function of cluster'size and the stationary porosity presents a power law and a linear dependency, respectively.

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