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Correlation between morphology and transport properties of composite films: Charge transport in composites

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Abstract

Metal/dielectric composite films consisting of metal objects located in dielectric matrix are investigated by computer simulation. The complete computer experiment is devoted to the study of correlation between structural properties and electrical characteristics of composite films. In the present analysis transport properties of films are calculated near the metal–dielectric transition when the basic mechanism of charge transport is the tunnel effect. The conductivity of composite film is disseminated into individual percolation paths influenced by object arrangements in the composite film.

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1. Introduction

Thin composite films represent class of promising materials. Composite or often nanocomposite metal/dielectric structures consisting of metal (nano)particles embedded into dielectric matrix have received more and more attention in last years due to their optical, mechanical and electrical properties. Metal nanoparticles have unusual chemical and physical properties which make them attractive for applications such as catalysis, electronics, optics, and biotechnology [1]. Technologies used for the preparation of these films can be various chemical methods [2], thermal decomposition [3], the simultaneous thermal evaporation from two sources [4], the ion-beam sputter technique [5], pulsed laser deposition [6] and the plasma deposition techniques—simultaneous plasma etching and plasma polymerisation, plasma polymerisation of organometallic compounds or simultaneous plasma polymerisation and metal evaporation. For most technologies it was observed that the composite films contain nanometer sized metal particles with excellent uniformity, at least for small filling factors [5,7]. To prepare composite thin films with desired properties we have to both know the structure and have a method which allows manipulation of the film structure. The properties of the films are dependent on size, concentration, and spatial distribution of the particles [8].

In order to characterise the composite film itself and to predict its other physical properties, the film morphology must be investigated and the structural descriptors must be found. The goal of morphological analysis of composite films is to characterise the forms and spatial distribution of individual metal objects in the film, especially in films with small filling factors and the films near the percolation threshold. If the film is thin enough, it is possible to use either the projections or planar sections of composite structures as input data, both obtained from microscopy. Then one can process them by standard image analysis.

One of the most important properties of composite films is their electrical conductivity near their percolation threshold. Therefore, in our laboratories we started to perform simultaneous analysis of morphological and transport properties of composite films in order to find correlation between film structures and their electrical conductivity. As the theoretical approach to this problem leads to the nearly invincible difficulties, a computer experiment is used for this purpose.

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The present contribution is devoted above all to the study of transport properties of composite films. In the next future, the results of both morphological and transport analyses will be compared and searched for common features. The main task of this simultaneous analysis of composite films is to find correlation between film morphology and its electrical conductivity and in such a way to bring additional information for the statistical three-dimensional (3D) reconstruction of composite structures from two-dimensional (2D) images.

2. Model

The complete computer experiment consists of several stages—generation of composite structures, their morphological analysis, analysis of their transport properties, and a comparative analysis of film morphology and electrical properties.

First, several sets of simulated composite structures were prepared. Spherical metal objects with constant radii were generated in a 3D working area with typical parameters: $1000 \times 1000 \times 100$ to $1000 \times 1000 \times 500$ pixels with boundaries, pixel being the length unit in our model. The principal technique of object simulation was the static hard-sphere model [11] with the basic parameter called diffusion zone $DZ \in \langle 0, DZ_{max} \rangle$. The objects are generated randomly not touching each other and the diffusion zone is the minimum distance between edges of objects. This model parameter determines the degree of arrangement of metal objects located in the dielectric matrix, the structures with higher diffusion zones are more ordered. The value of DZ_{max} is given by a number and dimensions of metal objects in the generated composite structure. In order to guaranty the reasonable precision of our results, the typical number of objects in the model varied between 1×10^3 and 1×10^4. An example of prepared sample can be seen in Fig. 1. In some simulations the simple hard-sphere model is not sufficient. In this case several more sophisticated methods of the film generation were suggested in order to make better fit to various types of experimental data [12].

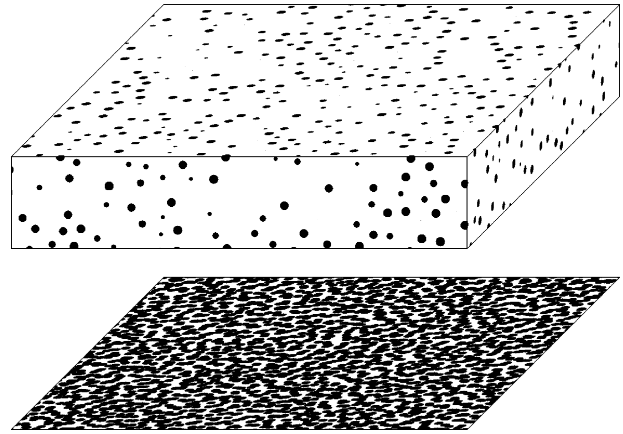

Fig. 1. Image of composite films, its section and projection. Diffusion zone maximal ($DZ/DZ_{max} = 100\%$).

The main task of the present computer experiment is to find method for analysis of transport properties in 3D composite structures. However, the 3D structures are not suitable for imaging of derived as well as for development of algorithms. Therefore, the artificial 2D analogy of composite films was used for this purpose. This type of model has the working area 1000×1000 pixels with boundaries. The objects are circular with constant radii and their surface distribution is given by hard-disk model with the same parameter DZ (see Fig. 2). Both types of models, 3D as well as 2D, were used in our simulations, but the results are demonstrated for 2D analogies of composite films only in the following figures. These analogies differ from the discontinuous metal films usually studied in thin film physics by other characteristics of metal objects—especially by their forms, although some transport processes are similar.

3. Results

The 3D model structures are used for the study of morphological properties of composite films. The input

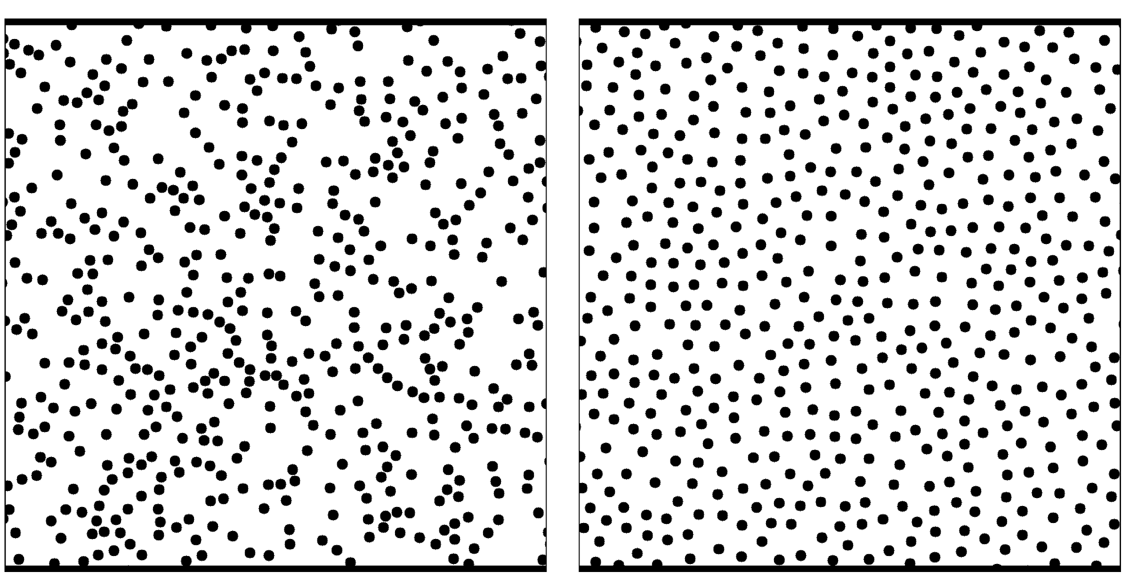

Fig. 2. Two-dimensional analogies of composite films. $DZ/DZ_{max} = 0$ (left) and 100% (right).