Morphology of Metal/Dielectric Composite Films – Thick Sections

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ABSTRACT

Thick sections of metal/dielectric composite films consisting of metal objects located in a dielectric matrix are studied by computer simulation. The complete computer experiment is devoted to the study of structural properties of composite films. One of parts of the computational study of composite films – introduction and usability of thick sections of composite films for their morphological analysis – is presented in the contribution.

INTRODUCTION

Morphological analysis of metal/dielectric composite thin films is important both for the characterisation of the films themselves and for the analysis of their properties. These interesting films represent class of promising materials. Composite metal/dielectric films consisting of metal particles embedded into an oxide or polymer matrix have became more and more attractive in last few years because of their interesting properties. Composite material can be obtained by embedding metal particles into a matrix of dielectric film. It can be achieved among other methods by thermal evaporation [1], ion-beam sputter deposition [2] or plasma deposition techniques (e.g.[3]).

There are three possible structures of the metal containing polymer or oxide films depending on the filling factor:

• low filling factor: the metal particles are completely insulated from each other and are embedded in a polymer matrix;
• medium-sized filling factor (critical filling factor): near the critical filling factor the metal-dielectric transition can be observed and metal objects form a percolation structure with interesting behavior;
• high filling factor: the metal film with polymer inclusions.

To make a proper analysis of prepared composite films a suitable technique for their structural description must be introduced. Theoretical approach to the problem often leads to the nearly invincible difficulties [4]; therefore, a computer experiment would be more suitable for that purpose.

In our contribution, a computer experiment for testing of methods, which are convenient for partial reconstruction of three-dimensional information from two-dimensional images, i.e. film projections, sections, and newly introduced thick sections, is described. Our main tasks were to gain information about the spatial distribution of objects in the film. For the characterisation of spatial distribution of objects in two dimensions – in discontinuous metal films – numerous morphological methods are known. Some of these methods, e.g covariance or Voronoi tessellation, can be applied to composite films with small amount of metal, too. However, near the percolation threshold these methods partially lose their sensitivity and new or at least modified morphological methods must be suggested. We introduce new method here, so called thick sections and we try to use the Voronoi tessellation on it. In the contribution these methods are analysed.

MODEL

We got ready a few sets of simulated composite films. The proportions of 3D structures are 1000×1000×500 pixels (x, y and z directions) plus borders in order to minimize boundary effects. One pixel is set as a length unit for spatial distribution of objects. One pixel corresponds approximately to 0.1 nm in our models. The generated objects are spherical and have constant diameter in accordance with many experiments. The number of generated objects is determined by the choosen filling factor (0.25 in this contribution). Thickness of the sec-

Figure 1: Image of composite film with spherical objects of constant diameter and filling factor 0.25.
tions and distance between objects themselves or objects and section boundaries are represented by real numbers.

For the generation of the spatial distribution of objects, the ‘hard-sphere technique’ was used: the objects are generated randomly not touching each other and the minimum distance between edges of objects is the model parameter called the ‘diffusion zone’ $DZ_{<0,DZ_{\max}}$. With the help of this parameter, it is possible to influence the randomness of spatial distribution of the objects. The structures with higher diffusion zone are more ordered.

**THICK SECTIONS**

Many methods, e.g. the Radial Distribution Function (RDF) [5], the Distribution of Nearest Neighbours (DNN) [6], Covariance (CO) [7], Chord-Length Distribution of Light segments (CHLD-L) [8], Quadrat Counts (QC), Wigner-Seitz Cells (WS) [9] often mentioned as Voronoi tessellation [10], characterizing the spatial distribution of objects in 2D are preferred in thin film physics. All the methods mentioned have been commonly used in 2D problems. We are trying to apply the WS in the case of 3D reconstructions of composite films by the help of thick sections [4].

Use of projections of composite films with higher filling factors is difficult for 2D analysis because of overlapping objects in the projection plane. Sections of the studied structures are suitable for morphological analysis but mostly hardly to obtain experimentally. These disadvantages can be overcome by using of the thick sections and subsequently the morphological analysis of their projections (see Figure 2). In our computer experiment, we studied the dependence of the distribution of object radii on the thickness of the thick section (see Figure 3) to see the difference between thick sections and projections or sections. The dependence of the radii distribution on the thickness of the thick section is obvious. It can be seen that the frequency function moves to the maximal radius of the objects with increasing thickness of the thick section. It is caused by the increasing number of spheres which are projected with the full diameter in the projection of the thick section. On the other hand, the number of objects intersected by the boundary planar planes of the thick section remains constant despite of changing the thickness of the section as well as the number of objects in the bulk.

![Figure 3: Distributions of object radii in thick sections of different thicknesses, pixel being the unit of the radius and $d$ denotes thickness of the thick section in pixels. Radius of the spheres equals 10 pixels.](image)

It seems to be here a limitation for usable thickness of the thick section, which is probably double diameter of the spherical objects embedded in the matrix. In the case of thicker sections than double diameter thickness the same disadvantage as in case of the projections of composites films appears – many object images are overlapped and it makes the analysis difficult, perhaps impossible.

When we apply analysis by means of WS cells we can obtain interesting results. Figure 4 shows WS analysis of the projections of the thick sections (thicknesses of thick sections equal the radius of objects) of two composite structures with different diffusion zones, first $DZ = 0$ pixels or $DZ = 5$ pixels. When we compare distributions of areas of WS cells of these structures, one can see the differences between random structure with zero diffusion zone and more ordered structure with higher $DZ$. The distribution function is narrower in case of more ordered structure.
Figure 4: Two-dimensional projections of thick sections of structures with different diffusion zones and corresponding distributions of WS cell areas. Top – diffusion zone = 0 pixels, bottom – diffusion zone = 5 pixels. Thicknesses of thick sections equals – the radius of the objects. Relative frequency on the value axis is in arbitrary units, value of WS cell areas on the series axis are in quadrat pixels.

CONCLUSION

A new method – thick sections – for study of spatial distribution of objects in composite films was introduced and tested. It seems to be very useful in case of dense structures. The dependence of the radii distribution of objects on thick section thickness is shown. There exists the upper limitation of the usable thickness of the section – it seems to be double diameter of the spherical objects. The projections of thick sections can be used e.g. for WS analysis of 2D information. The distribution of areas of WS cells can indicate the degree of orderliness of the composite structure in the case of thick sections.

ACKNOWLEDGEMENTS

The work is a part of the research plan MSM0021620834 that is financed by the Ministry of Education of Czech Republic. The authors acknowledge the support of the Czech Academy of Sciences, project IET400720409. The authors R. H. and M. S. acknowledge the support of the Grant Agency of Charles University Prague, Grant GAUK-237/2005. The authors acknowledge the support of the project LC06041.

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