ROLE OF PROJECTIONS AND SECTIONS IN MORPHOLOGICAL ANALYSIS OF COMPOSITE FILMS[1]

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The paper is devoted to a computer study of morphological properties of thin composite films. A computer experiment was suggested for testing of suitable methods of morphological analysis of the films. A computer model was prepared to study the 3D structural properties on the basis of 2D projections or sections. A special attention is devoted to covariance method.

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1 Introduction

In the last few years a growing attention of scientific community is devoted to various kinds of composite films, which seem to be very promising for next development of materials with new and well-defined properties. Especially, nanocomposite materials became very new and popular lately. They facilitate to produce films with the hardness of diamond [1] and possibly even harder. Morphological analysis of composite or nanocomposite thin films is important not only for a film characterization but also for an analysis of the film properties.

We will suppose composite films consisting of two solid phases, in the next parts. They can be formed e.g. of metal islands in a dielectric matrix. This type of composites can be produced among other methods by thermal evaporation [2], ion-beam sputter deposition [3] or plasma deposition technique [4].

The main goal of the paper is to show a proper method for the morphological analysis of three-dimensional (3D) composite structures. We wanted also to evaluate information acquired from sections or projections of the composite films by means of the chosen method for morphological analysis.

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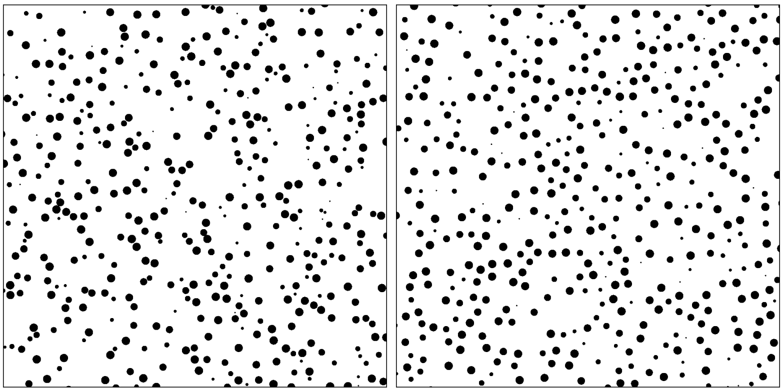

Fig. 1. Random sections of structures simulated with filling factor 0.1 for $DZ = 0$ (left) and DZ_{max} (right).

2 Model

In order to study the ability of present morphological methods to describe the spatial distribution of objects in the composite film, a simple computer experiment was prepared. Our model of composite structure uses working region 2000×2000×500 units (x, y and z directions) plus 10 % boundary regions in all directions; pixels being the length units in our model. The number of generated objects is always the same - 5000, and the spherical form of objects is assumed in accordance with many experiments. The sphere diameters were determined by the chosen filling factor of the film (in the range 0.05 to 0.35) and were kept constant in one set of simulated data. The hard-sphere technique was used for the generation of the spatial distribution of objects. The objects were generated randomly and the minimum distance between edges of objects is a model parameter called the 'diffusion zone' $DZ \in < 0, DZ_{max} >$. By means of this parameter, it is possible to influence the degree of arrangement of the objects; i.e. the structures with higher diffusion zones are more ordered. However, the same statement holds even for the filling factor - the systems with larger diameters of objects and thus with higher filling factor but with the same diffusion zones are more ordered, too. These two influences combine together making the discussion of results of simulation difficult.

Two types of images can be prepared from the generated composite structures - sections parallel to the (x, y) plane and/or projections of the three-dimensional structure on the substrate plane. The thickness of the composite film t is another parameter of our model.

Examples of images of generated structures are shown in Figs. 1 to 3. From these examples, it can be seen that while the analysis of film sections can be performed for the whole range of parameters of simulations, the information in the projections is very quickly destroyed with increasing film thickness. In order to express this dependence quantitatively, the more detailed morphological analysis of obtained images must be

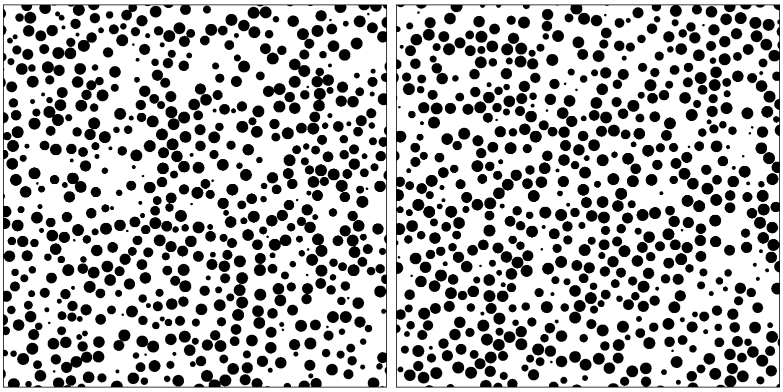

Fig. 2. Random sections of structures simulated with filling factor 0.3 for $DZ = 0$ (left) and DZ_{max} (right).

carried out.

3 Morphological analysis of sections

In order to analyze pictures that consist of separated objects, one can use many of the well-known morphological methods. However, the discrete objects start to coalesce for certain values of parameters in case of projections as it is seen in the Fig. 3. This fact narrows the spectrum of morphological methods applicable for the both projections and sections. We chose the covariance method, which gives very good results in case of two-dimensional (2D) films because it gives information at the same time about filling factor of the film (the starting value for $h = 0$), about mean diameter of objects (slope of the covariance function in the beginning), about degree of arrangements of structure (presence, number and heights of peaks), about mean distance of objects (position of the first minimum and the next maximum). Nevertheless, this method used for 3D films is naturally more sensitive in case of sections than for the projections [5].

We have applied the covariance method on the pictures of section of composite film. The results are depicted in the Fig. 4. In the upper part we see covariance functions for various sections of composite films. Parameter is here the filling factor. Bottom, there are compared covariance functions every time for two extreme values of diffusion zones. The filling factor is still a parameter.

4 Morphological analysis of projections

The previous procedure was used for the analysis of projections of composite films, too. We used the covariance method on the pictures of projections. In the Fig. 5 we can see covariance functions for various film thickness when the filling factor equals 0.2 and the diffusion zone is as large as possible, it means highly ordered structures. Seeing that a

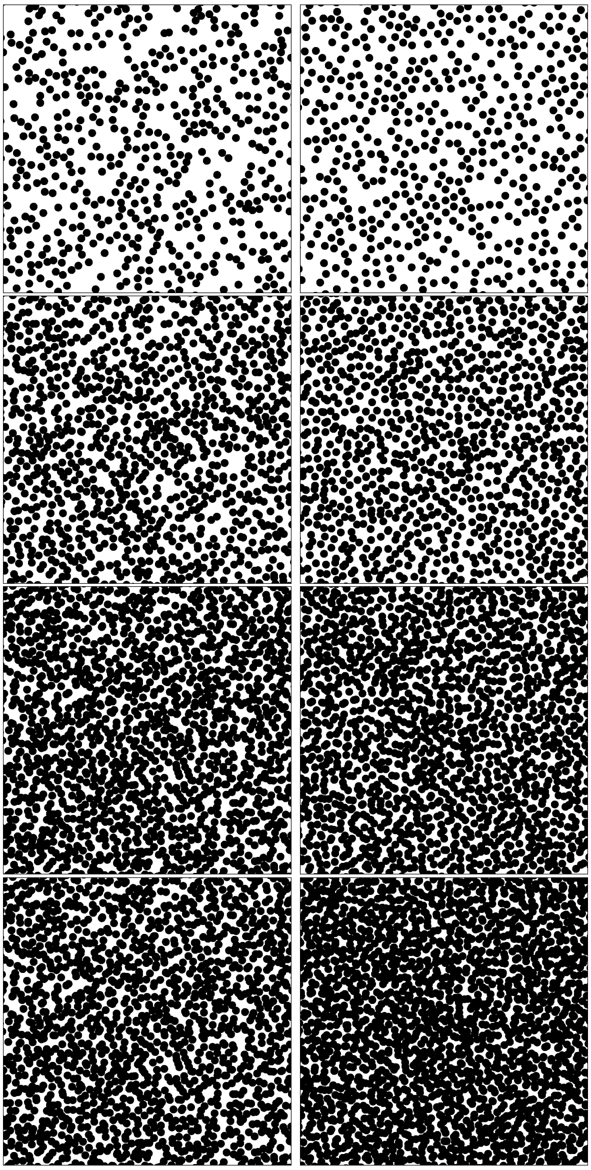

Fig. 3. Projections prepared from two structures simulated with filling factor 0.2 and diffusion zones $DZ = 0$ (left) and $DZ = DZ_{max}$ (right). The other parameter is the film thickness t increasing from 50 to 200 (downwards).

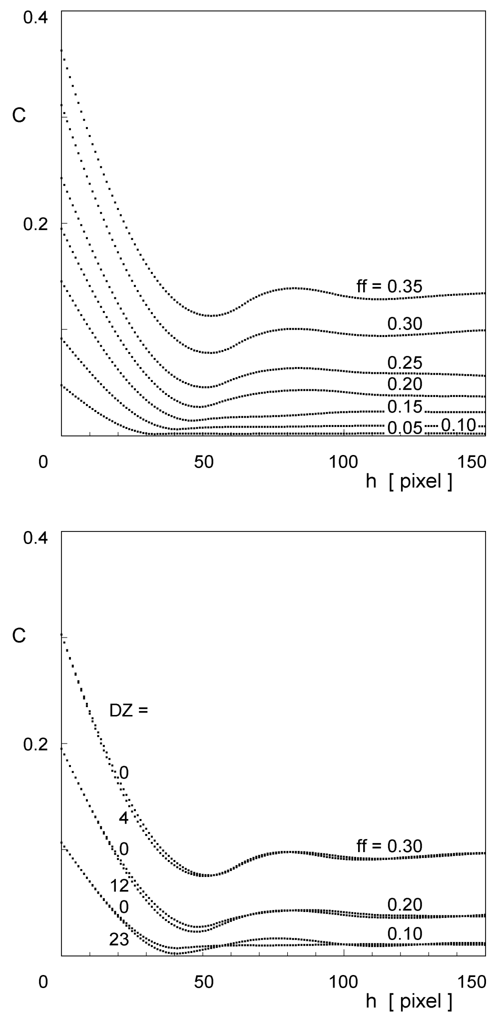

Fig. 4. Covariance functions of sections. (Top) diffusion zone $DZ = 0$, parameter: filling factor *ff*. (Bottom) filling factors *ff* $= 0.1$, 0.2 and 0.3 and two extreme values of diffusion zone: 0 and DZ_{max}.

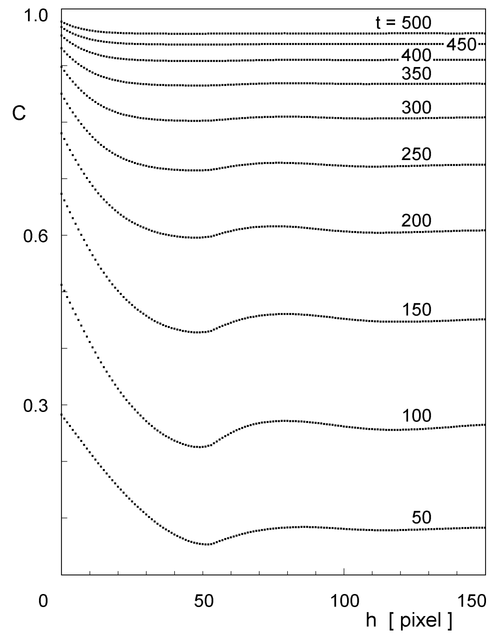

Fig. 5. Covariance functions of projections: filling factor $ff = 0.2$; diffusion zone $DZ = DZ_{max}$; parameter: thickness of the composite film t.

comparing of the covariance curves gets only qualitative information (see Fig. 4 bottom), we have tried to suggest a special quantities to describe the form of curves. Two of them had proved to be good for a description of the degree of arrangement of the composite structures: (i) the relative depth of the first minimum of the covariance function $C(h)$ - we denote it as $F1$, and (ii) the relative height of the second maximum denoted as $F2$. Both quantities are normalized to the value $C(\infty)$.

In the Fig. 6 is seen the dependence of the covariance quantity $F1$ on the composite film thickness both for non-arranged and completely arranged structures always for three values of filling factor. The quantity $F1$ differs for random and ordered structures in case of thinner films and for small filling factors. In this case $F1$ indicates the degree of arrangements of the structure.

5 Discussion

Results of our simulations show that the covariance method is suitable to characterize 3D structures by means of sections and/or projections. We have concluded that the covariance function is sensitive to parameters of composite films, i.e. to filling factor ff and to degree of arrangement simulated by diffusion zone DZ.

In case of sections, a certain degree of sensitivity is kept in the whole range of simulation parameters. E.g. the quantity $F1$ reaches the following values for curves in Fig. 4

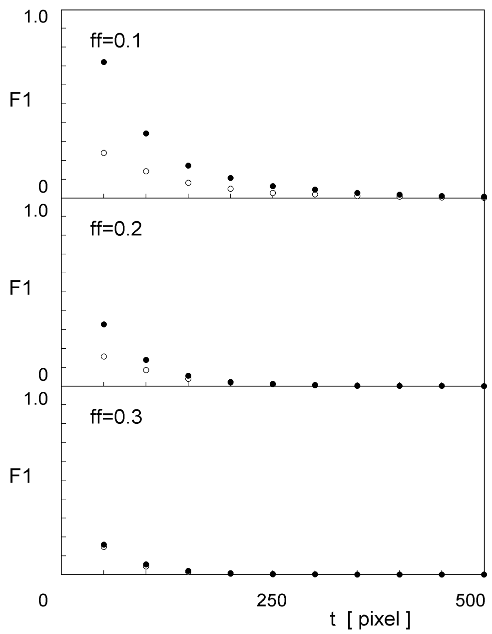

Fig. 6. Covariance functions of projections: dependence of the covariance feature $F1$ on the film thickness t for non-arranged structures generated with $DZ = 0$ (light circles) and for completely arranged structures with $DZ = DZ_{max}$ (dark circles)

bottom: 0.258 and 0.813 for *ff*=0.1; 0.288 and 0.402 for *ff*=0.2; and 0.181 and 0.195 for *ff*=0.3. Nevertheless, the sensitivity decreases with increasing filling factor because the original 3D structure itself with diffusion zone $DZ=0$ is enough ordered for higher filling factors.

On the other hand the projections have limited information capacity since the images are getting worse to analyze (see Fig. 3) with increasing film thickness. In the same manner the curves in Fig. 5 behave. They quickly get straight when the thickness of the film increases, and in the same way they lose their information stored. This behaviour we observed for all filling factors studied. The process speeds up with the growing filling factor.

The properties mentioned above are quantitatively depicted in the Fig. 6 for the quantity $F1$. Practically the same behaviour shows the quantity $F2$, only its sensitivity is lower.

From the practical point of view, the information obtained from projections is more easily accessible. For instance, the most common input for subsequent computer analysis of composite films consisting of metal islands in dielectric or polymer matrix, is a micrograph of the film from TEM, i.e. a projection of the film. To gain a section of it is very difficult even if not possible. From those reasons, the analysis of information capacity of projections is very important.

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