

Computational Study of Composite Films

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Abstract : Composite and nanocomposite films represent the class of promising materials and are often objects of the study due to their mechanical, electrical and other properties. The most interesting ones are probably the composite metal/dielectric structures consisting of a metal component embedded in an oxide or polymer matrix. Behaviour of composite films varies with the amount of the metal component inside what is called filling factor. The structures contain individual metal particles or nanoparticles completely insulated by the dielectric matrix for small filling factors and the films have more or less dielectric properties. The conductivity of the films increases with increasing filling factor and finally a transition into metallic state occurs. The behaviour of composite films near a percolation threshold, where the change of charge transport mechanism from a thermally-activated tunnelling between individual metal objects to an ohmic conductivity is observed, is especially important. Physical properties of composite films are given not only by the concentration of metal component but also by the spatial and size distributions of metal objects which are influenced by a technology used. In our contribution, a study of composite structures with the help of methods of computational physics was performed. The study consists of two parts: -Generation of simulated composite and nanocomposite films. The techniques based on hard-sphere or soft-sphere models as well as on atomic modelling are used here. Characterizations of prepared composite structures by image analysis of their sections or projections follow then. However, the analysis of various morphological methods must be performed as the standard algorithms based on the theory of mathematical morphology lose their sensitivity when applied to composite films. -The charge transport in the composites was studied by the kinetic Monte Carlo method as there is a close connection between structural and electric properties of composite and nanocomposite films. It was found that near the percolation threshold the paths of tunnel current forms so-called fuzzy clusters. The main aim of the present study was to establish the correlation between morphological properties of composites/nanocomposites and structures of conducting paths in them in the dependence on the technology of composite films.

Keywords : composite films, computer modelling, image analysis, nanocomposite films

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