## The Deformable and Strength Characteristics of Nanocomposites Improving

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Abstract. Mechanical properties of composites and nanocomposites have been considered in the assumptions of linear elasticity. To describe the nanoscale contact between matrices and inclusions on the interface surface, the conditions of ideal contact and non-classical Gurtin-Murdoch conditions have been implemented. The influence of shapes and relative sizes of inhomogeneities and matrices of representative volumes on the effective elasticity modulus of nanocomposites has been treated. Matrices in the form of cube and cylinder of finite sizes and inhomogeneity in the form of spheres and fibers have been considered. Finite element-based calculation models have been generalized to composites with distributed nanoinclusions of random and ordered orientation. The resulting models create the informative base for nanocomposites synthesis technologies with improved deformable and strength characteristics.

#### **Problem formulation**

The actual issues of the elasticity linear theory include the study of elastic and mechanical properties of modern technological and innovative nanocomposite materials. The validity of the simulation results for such materials requires appropriate mathematical models that adequately describe the structures of nanoscale inclusions. If the analysis focuses on the interaction of atoms in nanomaterials, then the corresponding models should be based on the quantum mechanics principles. Nevertheless, if the research aimed to model the average mechanical characteristics, average deformations or effective elastic modules, then the continuous mechanics approaches could be successfully applying to ensure effective estimations. It should be noted, that three-dimensional configurations were analyzed mainly with the assumption of the presence of spherical particles in the nanocomposite. For these forms of nanoinhomogeneities, it has been proved that the properties of interfacial surfaces could significantly affect both elastic fields and effective modules of composite materials. The multilevel approach is one of the main directions of modern mechanics of nanoscale materials, aimed to expand the classical continuum mechanics scope due to combining its basic theoretical principles with the effects observed at the molecular level. For the calculating problem of the effective materials properties in the presence of the intermediate layer between contacting surfaces has given enough attention. The issues of determining the effective modules of composites and nanocomposites taking into account the surface effects influence and in the presence of ordered inclusions systems in the representative cells remain relevant.

#### **Analysis of Publications**

Recently, publications devoted to the determination of the mechanical properties of nanocomposites have been treating the effects of the interfacial surfaces presence, which could significantly affect both elastic fields and effective modules of composite materials. The Gurtin-Murdoch model [1] of the elastic surface has been often used in recent publications on nanocomposites [2, 3]. This model

#### Outcomes

Computational models for a wide class of three-dimensional nanocomposites have been created, which adequately reflect the elastic properties of nanostructures and could be able for efficient numerical modeling. Closed systems of boundary integral equations of three-dimensional static issues on the behavior of elastic composites with nanoscale inhomogeneities have been obtained. The gained models have provided numerical research and efficient prediction of mechanical properties of three-dimensional matrix nanocomposites for the full range of structure parameters. To describe the effects at the nanolevel, both the classical model and the Gurtin-Murdoch model, which includes both surface tension and surface stiffness, have been adopted. To achieve high accuracy of numerical analysis with the help of developed nanoscale models, the methods of boundary and finite elements have been improved to consider the non-canonical shape of nanoscale particles and nonclassical interphase conditions. In algorithms of boundary methods and finite elements, the finite system of linear algebraic equations concerning to interphase displacements and forces has been obtained after special regularization and adapted discretization of boundary integral and variational equations. The proposed models and algorithms of computer simulation allow to provide numerical analysis of three-dimensional static issues of single nanoinclusion of different shapes (granule, fiber) and classical and non-classical conditions of contact with the surrounding matrix; three-dimensional problems on static interaction of a finite number of nanoscale inclusions in the matrix; study of ordered inclusions. Research of inclusions in the form of spheres, and carbon nanofibers allow us to determine the effective elastic parameters of three-dimensional matrix composites with nanoinclusions. The obtained models create the informative basis for technologies of synthesizing nanocomposites with improved deformation and strength characteristics, in particular with the pronounced anisotropy of elastic properties.

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