2021 IEEE 2nd KhPI Week on Advanced Technology

(KhPI Week)

CONFERENCE PROCEEDINGS

September 13 - 17, 2021

Kharkiv, Ukraine

2021 IEEE 2nd KhPI Week on Advanced Technology (KhPI Week)

IEEE Catalog Number: CFP21Z72-ART
ISBN: 978-1-6654-1205-6

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CONTENTS

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BoundaryCalculation Models for Elastic Properties Clarification of Three-dimensional Nanocomposites Based on the Combination of Finite and Boundary Element Methods

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***Abstract* — Object-oriented models have been developed for the wide class of three-dimensional nanocomposites that adequately reflect the elastic structures properties and are applicable for efficient numerical modeling. Closed equations systems have been obtained with the provision of boundary-integral and variational formulations of three-dimensional static problems on the behavior of elastic materials with inhomogeneities of nanoscale. The obtained models allow to effectively predict the three-dimensional matrix nanocomposites mechanical properties for the full class of structure parameters. To characterize the effects at the nanoscale, both the Gurtin-Murdoch and classical model have been adopted, which includes the surface tension and surface stiffness.**

Keywords* — *nanocomposites; representative three-dimensional elements; spherical inclusions; finite element method; boundary element method

I. INTRODUCTION

Nanocomposites are widely used in practice as responsible internal and covering elements of engineering structures and systems. Their contribution to significant strengthening and maintaining the lightness and reliability of objects is crucial for treatment. Therefore, it is important to develop new effective methods for treating the nanomaterials properties in all their diversity due to the dispersion of material components, the distribution of nanoparticles, the shape and order of nanoinclusions and nanofibers.

Computer modeling and computational experiment are powerful measures for such research by providing uniform parameterization of the nanocomposites behavior in the wide range of their material, geometric and surface features. Furthermore, numerical simulation could in many cases significantly optimize the physical experiment based on information from numerical analysis with the volume decreasing, cost and time of experimental research.

The accuracy of the results of numerical calculations has been based on the correct choice of models or theories that would adequately describe nanoscale structures. If the analysis focuses on interatomic interactions or chemical reactions in nanomaterials, then it has been started from models of quantum mechanics or molecular dynamics.

However, if the purpose of the analysis is to study the impact of global mechanical interactions, in particular on deformability, static and dynamic load transfer mechanisms or effective stiffness parameters, then the approaches of continuous mechanics could be endowed with greater productivity. The implementation of combined models of continuum mechanics and molecular dynamics could be also perspective for interlevel analysis. Improvement of these models should be achieved taking into account the physical and spatial-surface specificity of the constituent nanocomposites.

The boundary element method (BEM) is one of the most common numerical methods used in various engineering fields. BEM is usually applied to boundary value problems, formulated in the form of differential equations with partial of conducting the field experiment based on the leading data from numerical analysis.

The gained models form the informative basis for synthesizing nanomaterial technologies with advanced deformation and strength characteristics, in particular with the pronounced anisotropy of elastic properties.

ACKNOWLEDGMENT

The research is partially supported by the “Program for the State Priority Scientific Research and Technological (Experimental) Development of the Department of Physical and Technical Problems of Energy of the National Academy of Sciences of Ukraine” (#6541230).

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