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MULTISCALE AND MULTYPHYSICS MODELING OF FILLED COMPOSITES, DESIGN VALIDATION OF THE MODELS AND UNCERTAINTY IN THE MODELLING

*** S. Lurie[1], D. Volkov-Bogorodsky[2], N. Tuchkova[3] and V. Zubov[3]**

[1] Inst. of Applied Mechanics
Russian Acad. of Sciences
Leninskii pr. 32 a, 119991,
Moscow Russia
lurie@ccas.ru

[2] Inst. of Applied Mechanics
Russian Acad. of Sciences
Leninskii pr. 32 a, 119991,
Moscow Russia
v-b1957@yandex.ru

[3] Dorodnicyn Comp. Centre of
Russian Acad. of Sciences
Vavilov st. 40, 119334
Moscow GSP-1, Russia
zubov@ccas.ru
tuchkova@ccas.ru

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ABSTRACT

The physical problem of modeling for materials enhanced with nanofiller is associated with the significant length of interphase layer that dominate the structure and properties of the media. The consistent and yet accurate multiscale model of material media with a spectrum of cohesion and adhesion interactions is developed using the variant of the kinematics variation principle. The sequential description of kinematics of the solid media with a range of different internal structures is described across the length scales by a series of physical models, i.e. model of porous media, turbulence and twinning models, model of an interphase layer and unit cell model for composites with spectrum of adhesion and cohesion interactions[1].

The mathematical problems of modeling are associated with investigations of the structure solution for the boundary value problem of the gradient theory with the higher order governing equations than those in the classical theory of elasticity. The set of constitutive relations is established and the corresponding consistent boundary-value problems are formulated. The proposed general model allows analyzing various length scale effects, e.g., cohesive interactions; surface effects (surface tensions, capillarity etc.) in both volume and surface of the media. The models have provided the understanding of important non-classical effects observed in the mechanics of materials, e.g. nonsingular stresses, Barenblatt hypothesis about existence of the cohesion fields; theoretical hypothesis about the relationship between the length of the cohesion interaction zone and parameters of fracture mechanics[2]; an effect of material strengthening by micro and nano- particles at the constant volume fractions [3-5] and others. The proposed formulation and mathematical approach to the constitutive equations is presented in a consistent way. Generalized Pascal equation for a surface tension pressure, generalized Young law for the description of wettability is established as a result of multi-physics and analytical investigations of the corresponding material problems. The generalized Eshelby's problem is extended on the higher-order

continuum theory of the mediums, which take into account the specific properties of interphase layer for advanced composites with micro- and nanoscale inclusions.

Numerical modeling is carried out by a block method [6]. Design validation studies have been carried out by computer runs out of the model and consistency checks of error log. The identification problem of the model parameters was a challenge. A problem of finding model parameters that corresponds to experimental data is formulated as a variation problem so as to minimize the cost function and uncertainty caused by the modeling approach. For validation of the numerical algorithm the following mathematical and numerical problems are solved:

- general representation of displacement field through auxiliary vector potentials for gradient models is established on the basis of general Neuber-Papkovich concept;
- computational algorithm for predictions of force and moment characteristics of media contact problem, computational algorithm and algorithm for establishing a block system of the linear equations on a basis of the functional of the least squares method and modified functional.

An accuracy and reliability of the modeling approach has been validated by predict some basic mechanical properties of a polymeric matrix reinforced with nanoscale particles/fibres/tubes (including carbon nanotubes) as a function of size and dispersion of nanoparticles. The problem of homogenization is numerically solved with the aid of the special analytical-numerical method and effective mechanical properties of the filled composite were found across the length scales. The asymptotic average solution for gradient model was obtained on the base of the procedure of asymptotic homogenization for composite materials with periodic structure in framework of the gradient model of interphase layer.

The computer programming problem of modeling is associated with elaborating of the specific numerical tools for modeling of the boundary contact problems of the multicomponent solid bodies with complex local stress-strain states changing exponentially as well as predictions of specific analytical approximations, which is predicted from the equations and structure of the common solution.

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