Modelling of nanocomposites by using the effective particle concept and the boundary element method

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Abstract

The paper deals with the numerical homogenization of polymer/clay nanocomposites. It is known that stacks of parallel clay sheets, which can constitute the reinforcement structure, can be modelled as effective particles. For relatively small volume fraction of the reinforcement the effective particles can be considered as isotropic. On the other hand, for larger values of the volume fraction the particles should be anisotropic. In most of available articles, analytical methods or the finite element method (FEM) are applied. In this work the application of boundary element method (BEM) is considered. Two-dimensional numerical models are analysed, involving both cases of the effective particle: the isotropic one, and the anisotropic one as well. The matrix is modelled as isotropic. The problem is solved by using a special formulation for plates containing many identical inclusions. As kernels of boundary integrals for the isotropic subdomains the Kelvin solutions for plane elasticity are applied, and for anisotropic inclusions fundamental solutions obtained by the Stroh formalism will be used. Results of preliminary research related to isotropic effective particles confirm the validity of the method.

Keywords: anisotropy, boundary element methods, composites, homogenization, material properties, microstructures

1. Introduction

Polymer/clay nanocomposites are characterized by enhanced mechanical properties at low weight fractions of reinforcement in comparison to other types of composites. The reinforcement particle structure can be composed of exfoliated clay sheets or stacks of parallel nanoclay sheets. During the design of structures the knowledge of homogenized properties of composite materials are required. The properties can be determined by applying analytical, empirical or numerical methods. The most popular ones are: analytical formulas based on the Mori-Tanaka approach (M-T), the semi-empirical Halpin-Tsai method (H-T) and analysis of a representative volume element (RVE) by the finite element method (FEM). In recent years many papers has been published on this problem. A short chronological review of the articles is given below.

Wang and Pyrz in [11] presented the theory and formulas for the prediction of the overall moduli of layered silicate-reinforced polymeric nanocomposites. Formulas for the moduli of composite materials reinforced with transversely isotropic spheroids were derived using the M-T method. These formulas were used to examine the influences of the anisotropy and aspect ratio of the transversely isotropic spheroids on the overall bulk modulus and shear modulus of the composite materials. In the second part of the cited work [12] the authors applied their formulas to analysis of various montmorillonite silicate-reinforced polymeric nanocomposites. Sheng at al. [9] applied a multiscale modeling strategy, taking into account the hierarchical morphology of the polymer/clay nanocomposites, to the prediction of apparent properties of the materials. The clay particles can have the form of exfoliated clay sheets of nanometer level thickness or stacks of parallel clay sheets separated from one another by interlayer galleries of nanometer level height. It is shown that in the latter case the stacks can be represented by effective particles. Two-dimensional FEM simulations were performed involving isotropic effective particles. Hbaieb et al. [6] analyzed 2-D and 3-D FEM models of the polymer/clay nanocomposites with aligned and randomly oriented particles. They calculated effective Young's modulus in the axial direction and Young's modulus of the isotropic effective medium, accordingly to the analysed case. The results were compared to the M-T model. Figiel and Buckley [3] calculated elastic constants for the layered-silicate/polymer nanocomposite with intercalated morphology using the effective particle concept. Two methods were applied: 2-D FEM analysis and the M-T method. It was shown that the effective particle concept was valid if full anisotropy of the effective particle was taken into account. Górski and Fedeliński [4, 5], modelled 2-D RVEs of the nanocomposites by using coupled boundary and finite element methods (BEM/FEM). The matrix was modelled by the BEM, and the reinforcement by beam finite elements. The authors considered both aligned and randomly distributed particles. An influence of the volume fraction of the particles on homogenized Young's modulus in one direction was investigated. The results were compared to the M-T and H-T models, and to results obtained by other authors by 2-D FEM analysis. In the paper by Fedeliński et al. [2] different formulations of the BEM, for an analysis of composites containing rigid or deformable stiffeners and inclusions, were presented. The developed computer codes were used to compute homogenized elastic or piezoelectric material properties by analysis of 2-D RVEs or unit cells. One of the analysed materials was the polymer/clay nanocomposite reinforced with stacks of clay sheets.

The present work is a continuation of [8], where preliminary research concerning isotropic effective particles was performed. In this work also anisotropic particles will be considered in the BEM simulation of the nanocomposites. The two cases of effective particles will be compared.

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2. Numerical homogenization by the BEM

The BEM [1] is an effective method for the numerical homogenization of heterogeneous materials due to the discretization of the boundary only. In this work, the formulation for plate containing many identical inclusions (subdomains), presented by Yao et al. [13], is applied. All the constituents are linear-elastic. The matrix is considered as isotropic whilst the effective particles are isotropic or anizotropic. Respective kernels of boundary integrals are: the Kelvin solutions for the isotropic subdomains, and fundamental solutions obtained by using the Stroh formalism [10] for the anisotropic inclusions. Representative volume elements are modelled, with periodic boundary conditions imposed, assuming that macro-strain is known [7]. Homogenized elastic coefficients are calculated by means of macro-strains and stresses determined by using an averaging theorem, and the constitutive law on macro-scale.

3. Numerical example

Homogenized elastic constants of polymer/clay nanocomposite reinforced with intercalated particles are analyzed. The effective particles are modelled as rectangular inclusions. The RVEs are 2-D rectangles with many identical inclusions, in plane strain. Both the materials of matrix and inclusions are linear elastic and isotropic. Periodic boundary conditions are imposed. Geometry of typical RVE is shown in Figure 1. The results of homogenized Young's modulus E_{11} (in the horizontal direction), normalized with respect to the modulus of matrix E_m, for weight fraction of reinforcement W_c = 1÷6 %, obtained by the BEM are presented in Figure 2. Ten different models were analysed for each value of the weight fraction. The results are consistent with the ones presented by Sheng et al. [9]: experimental data and numerical results by the FEM analysis. More details on the analysed structures, results for remaining homogenized elastic constants and results of the analysis involving anisotropic particles will be presented in the full paper.

Figure 1: Geometry of a typical RVE

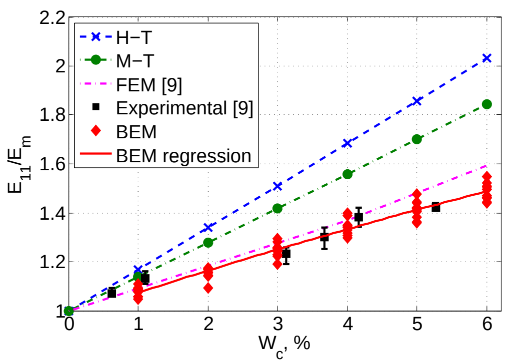

Figure 2: Normalized homogenized Young's modulus obtained by different methods

4. Conclusions

The preliminary results show that the BEM model can be applied to the evaluation of homogenized elastic moduli of polymer/clay nanocomposites. The results agree with analytical models, experimental data and numerical results presented by other authors. The analysis is efficient with respect to the number of degrees of freedom of numerical model and accuracy of results.

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