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New Method of Numerical Homogenization of Functionally Graded Materials

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Abstract

In the paper the method of numerical homogenization for FGM was proposed. It was based on the method shown in Vemaganti and Deshmukh (2006), in which the gradient heterogeneous microstructure is divided into homogenous slices. In the presented study the model was built with the use of 2D elements, with two linear material models of Young modulus $E=45$ MPa and 748 MPa distributed in sample volume in accordance to linear and normal distributions. Firstly the RVE was calculated. Then the numerical homogenization was carried out with the division of the heterogeneous sample into 4, 5 and 8 slices. The substitute material characteristics were calculated and implemented into sliced model. The numerical compression tests of the sliced and heterogeneous models and were compared. The conclusion was that the more slices we apply the more exact results we will get. This selection should be based on the accuracy we want to get and on the computational capacity we have. Also in this kind of modeling we cannot assess the stress distribution in microstructure.

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1. Introduction

Functionally graded materials (FGMs) are materials that comprise a spatial gradation in structure and/or composition, tailored for a specific performance or function. FGMs are not technically a separate class of materials but rather represent an engineering approach to modify the structural and/or chemical arrangement of materials or elements (by Udupa et al. (2014)).

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Computational models of materials and constructions allow to carry out complex simulations on the base of which it is possible to predict material properties, microstructural and macrostructural strength behavior and high strain rates interactions. It is also possible to simulate static and dynamic phenomena considering large deformations, contact effects, damage as well as heat transfer, changes in material properties in accordance to changes in deformations or temperature or phase transformations.

Computed simulations let us to carry out study impossible to make in experimental way (e.g. fast changing damage process in armor under detonation). Such methods are necessary especially for mult-variant tests, in which the aim is a selection of optimal construction or material structure for assessed implementation. It is also important due to the limitation of expensive and often dangerous experimental studies.

There are many methods of material microstructure modeling. One of them are idealistic models which use repeatability and symmetry of selected solids. The Kelvin tetrakaidecahedron built of regular hexagons and squares is an example of such idealistic structure (Kusner and Sullivan (1996)).

The assessment of repeatability and symmetry of the structure allows to reduce the numerical model dimensions and time of simulation, what is important for testing influence of various on material properties. Another well know idealistic structure is a Weaire-Phelan geometry (group of eight irregular polyhedrons with walls built of hexagons and pentagons (Sihna and Roy (2004))).

2D and 3D raster technique can be assumed as another interesting method of material structure modeling. It becomes more and more attractive with the increase in computational power. Such models are achieved on the base of raster pictures of real structures that are scanned with the use of e.g. diffraction methods. Euler sponge can be an example of such modeling (Mishnaevsky (2005)).

Also the models reflecting real structure in the most exact way. In this group we can find surface models built on the base of microscopic photo of the sample cross-section or solid models built on the base of computed tomography or Roentgen diffraction (Miedzinska *at al.* (2012)).

Other models are characterized with different level of idealization or simplification – these are so called phenomenological models. They are useful for research on influence of described geometrical properties on modeled materials properties (Jin *at al.* (2002), Li *at al.* (2005)). Those phenomenological models are often used in predicting specific properties of cellular media, such as porous or grain ones. The example of such property can be the auxetic behavior or shape memory phenomenon.

The simulation of a changeable pores distribution allows to study porous graded materials (Li *at al.* (2005), Szymczyk and Włodarczyk (2007)). In such methods it is possible to study the influence of pore distribution, such as pores connectivity, pores shape or orientation, on macrostructural material properties (Reiter and Dvorak (1998)).

For the real structures modeling also such methods as Voronoi or Dirichlet tessellations can be applied (Bruck and Gershon (2002)).

The level of model complexity can be very different in accordance to many factors such as researcher experimental background, which can be used at the initial phase as a source of data for model development and in the further phase as a model verification and validation data.

In the paper the new method of numerical homogenization of grain porous media with functionally graded and stochastic structure is presented. It was decided to implement raster statistical modeling method, in which pores distribution will be selected in a random way.

2. Representative Volume Element

Representative volume element (RVE) is the smallest, statistically homogenous volume which represents the properties of whole material. Macroscopic elastic modules cannot depend on RVE shape and dimensions. So in case of disordered distribution of defects the RVE must contain enough number of them, and the characteristic dimension of such defect l must be much more lower than characteristic dimension d of RVE – see Fig. 1. In the same time the RVE must be so small in comparison to researched sample, the we would be able to treat it as a material point in a macroscale. Summarizing the RVE must achieve the following condition (Lydzba and Rozanski (2014)):

$$l \ll d \ll L \quad (1)$$

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