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COMPOSITES THEORY AND PRACTICE

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NUMERICAL MODELLING OF FUNCTIONALLY GRADED COMPOSITE MICROSTRUCTURES IN TERMS OF THEIR HOMOGENIZATION

A new method of numerical homogenization for functionally graded composites (FGCs) was proposed in the paper. It was based on the method in which the gradient heterogeneous microstructure is divided into homogeneous slices. In the presented research, the model was built using 2D elements, with two linear material models of Young modulus E = 50 MPa and 750 MPa distributed in the sample volume in accordance with linear and normal graduation. The numerical homogenization was carried out by dividing the heterogeneous sample into 4, 5 and 8 slices. The substitute material characteristics were calculated and implemented into the sliced model. The numerical compression test results of the sliced and heterogeneous models were compared and the method error was calculated. The conclusion was that the more slices applied, the more exact results will be received. Selection of the number of slices should be based on the accuracy that is necessary for the global model to reflect the gradient properties of the structure and on the available computational capacity. A disadvantage of this modeling approach is the loss of ability to evaluate the distribution of stresses around the grains of individual phases in the microstructure.

Keywords: functionally graded composite, homogenization, numerical modeling

MODELOWANIE NUMERYCZNE MIKROSTRUKTURY KOMPOZYTÓW FUNKCJONALNIE GRADIENTOWYCH W ASPEKCIE ICH HOMOGENIZACJI

W artykule zaproponowano nową metodę homogenizacji numerycznej dla kompozytów funkcjonalnie gradientowych. Metoda ta została oparta na sposobie, w którym heterogeniczna mikrostruktura gradientowa jest dzielona na homogeniczne plastry. W prezentowanej pracy model został zbudowany z użyciem elementów 2D oraz dwóch liniowych modeli materiału o wartości modułu Younga E = 750 i 50 MPa, rozdystrybuowanych w objętości próbki zgodnie z rozkładem liniowym lub normalnym. Homogenizacja numeryczna została przeprowadzona poprzez podział heterogenicznej próbki na 4, 5 i 8 plastrów. Obliczone w ten sposób zastępcze charakterystyki materiałowe zostały zaimplementowane do modelu homogenicznego (plastrowego). Przeprowadzono testy numeryczne modeli heterogenicznych i plastrowych, których wyniki porównano i obliczono błąd metody. Wnioskiem z badań było stwierdzenie, że im więcej zastosuje się plastrów, tym dokładniejszy wynik zostanie uzyskany. Dobór liczby plastrów powinien być oparty na wymaganej dla modelu globalnego dokładności odzwierciedlenia właściwości gradientowych struktury oraz na dostępnej mocy obliczeniowej. Wadą takiego sposobu modelowania jest utrata możliwości oceny rozkładu naprężeń wokół ziaren poszczególnych faz w mikrostrukturze.

Słowa kluczowe: kompozyty funkcjonalnie gradientowe, homogenizacja, modelowanie numeryczne

INTRODUCTION

Functionally graded composites (FGCs) are materials that comprise spatial gradation in the structure and/or composition, tailored for a specific performance or function. FGCs 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 [1]. There are two types of graded structures which can be prepared in the case of FGCs, a continuous structure as shown in Figure 1a and a stepwise structure shown in Figure 1b. In the case of the continuous graded structure, the change in composition and microstructure occurs continuously with the position. On the other hand, in the case of the stepwise one, the microstructure features changes in a stepwise manner, giving rise to a multilayered structure with an interface existing between discrete layers [2, 3].

In the paper a new method of numerical homogenization of grain composite media with a functionally graded and stochastic structure is presented. The raster statistical modeling method, in which one phase distribution in a second one is selected in a random way was implemented.

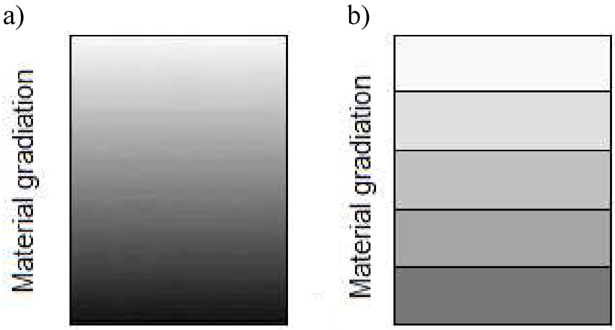

Fig. 1. Schematic diagram of FGC graduation concept [4]

Rys. 1. Schemat różnych typów gradacji w kompozytach funkcjonalnie gradientowych

NUMERICAL MODELING METHOD DESCRIPTION

There are many methods of material microstructure modeling. One of them is idealistic models which use the repeatability and symmetry of selected solids. The Kelvin tetrakaidecahedron built of regular hexagons and squares is an example of such a structure [5]. Assessing the repeatability and symmetry of the structure allows the numerical model dimensions and time of simulation to be reduced, which is important for testing the influence of various factors on the material properties. Another well-known idealistic structure is the Weaire-Phelan geometry (a group of eight irregular polyhedrons with walls built of hexagons and pentagons) [6].

2D and 3D raster techniques can be assumed as another interesting method of material structure modeling. They are becoming increasingly more attractive with the increase in computational power. Such models are achieved on the basis of raster pictures of real structures that are scanned with the use of, e.g. diffraction methods. The Euler sponge can be an example of such modeling [7] Moreover, models reflecting the real structure in the most exact way can be found. In this group we can find surface models built based on a microscopic photo of a sample cross-section or solid models built on the basis of computed tomography or Roentgen diffraction [8, 9].

Other models are characterized by different levels of idealization or simplification - they are so-called phenomenological models. They are useful for investigating the influence of described geometrical properties on modeled materials properties [10, 11]. Those phenomenological models are often used in predicting specific properties of cellular media, such as porosity or granularity. An example of such a property can be the auxetic behavior or the shape memory phenomenon. Simulating changeable phase distribution enables the study of porous graded materials [12, 13]. In such methods it is possible to study the influence of phase distribution on macrostructural material properties [14].

To model real structures, such methods as Voronoi or Dirichlet tessellations can also be applied [15].

The level of model complexity can vary depending on various 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 data for model verification and validation.

For the purpose of modeling functionally graded composites, a computer application was developed using VBA code. The elements in the model are drawn on the basis of assessed randomization (statistic distribution - linear or normal) using the application. For the drawings the Excel RAND function was used. The function RAND() returns a pseudo-random integral number, therefore the sequence will contain repeating series of numbers, if is long enough. Coupling random numbers, like in the Wichman-Hill procedure, allows numbers to be generated 10^{13} before repetition appears. In the case of some Diehard tests, the achieved results were incorrect because in older RAND functions the cycle of repeating numbers was too short. Finally, RAND() returns an evenly distributed random real number greater than or equal to 0 and less than 1. A new random real number is returned every time the worksheet is calculated. Examples of such drawings are shown in Figures 2 and 3.

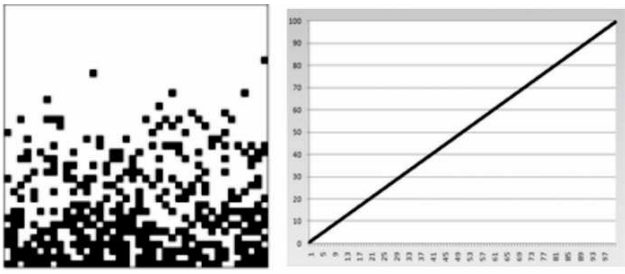

Fig. 2. FGC model with linear distribution of content of one phases on sample height

Rys. 2. Model kompozytu funkcjonalnie gradientowego o liniowym rozkładzie udziału jednej z faz na wysokości próbki

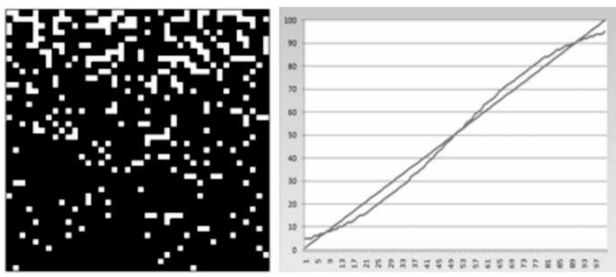

Fig. 3. FGC model with normal distribution(mean 50, standard deviation 30) of content of one of phases on sample height

Rys. 3. Model kompozytu funkcjonalnie gradientowego o normalnym rozkładzie (średnia 50, odchylenie standardowe 30) udziału jednej z faz na wysokości próbki

NUMERICAL HOMOGENIZATION METHOD

Selecting the homogenization method was based on the literature review. The most important are methods presented in [16, 17] where functionally graded material homogenization was proposed.

The general method of FGC homogenization is shown in Figure 4. The method is based on dividing the microstructure into relevant elements (here strips), for which substitute properties are calculated. Selecting the strip width to achieve the smallest error of homogenization is carried out based on local microstructure observation and calculations for series of models with different strip widths.

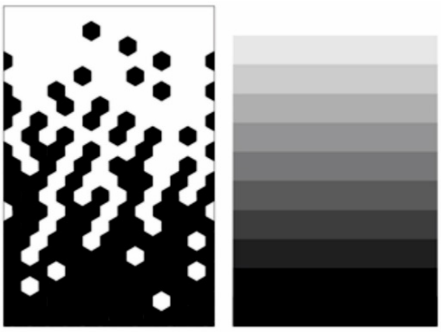

Fig. 4. Scheme of applied homogenization method [17]

Rys. 4. Schemat użytej metody homogenizacji [17]

To test the homogenization method presented above, the selected model of functionally graded composite with linear change in content of one of the phases on the sample height was used (Fig. 2). In the next step the FGC model with a normal distribution change in porosity on the sample height was tested (Fig. 3).

NUMERICAL ANALYSIS DETAILS

The uniaxial compression test was carried out by means of LS Dyna computer code. Two linear material models of Young modulus E = 50 and 750 MPa distributed in the sample volume in accordance with linear and normal graduation were applied (a Poisson's ratio of 0.3 was applied each time). The following boundary conditions were applied:

1. fixed nodes in the vertical (y) direction at the bottom of the sample
2. all fixed nodes in the direction perpendicular to the sample surface (z direction)
3. vertical compressing displacement of 1m/s at the top nodes of the sample.

The characteristic dimensions of each element in a model were 10×10 μm.

The following models were analyzed:

1. model before homogenization - 40×40×40 elements (LIN_ALL, STAT_ALL)
2. model after homogenization with the use of 1 strip - 40×40×40 elements (LIN_1, STAT_1)
3. model after homogenization with the use of 4 strips - 10×40×40 elements (LIN_4, STAT_4)
4. model after homogenization with the use of 5 strips - 8×40×40 elements (LIN_5, STAT_5)
5. model after homogenization with the use of 8 strips - 5×40×40 elements (LIN_8, STAT_8).

The models are shown in Figures 5-7.

On the basis of a non-homogenized structure, it was assumed that the material behavior is similar to a foam one. Therefore, the LS Dyna material model MAT_026_HONEYCOMB was used to model homogenized material behavior. The main use of this material model is for honeycomb and foam materials with real anisotropic behavior. Nonlinear elastoplastic material behavior can be defined separately for all normal and shear stresses. They are considered to be fully uncoupled [18].

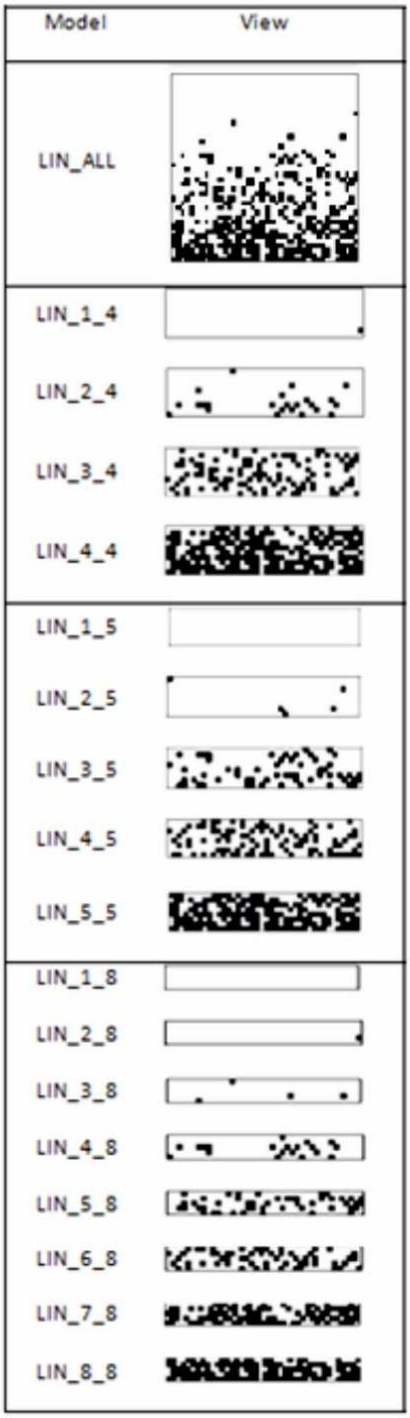

Fig. 5. Numerical models applied for homogenization method tests - models with linear distribution before homogenization

Rys. 5. Modele numeryczne użyte do testów metody homogenizacji - modele o rozkładzie liniowym przed homogenizacją

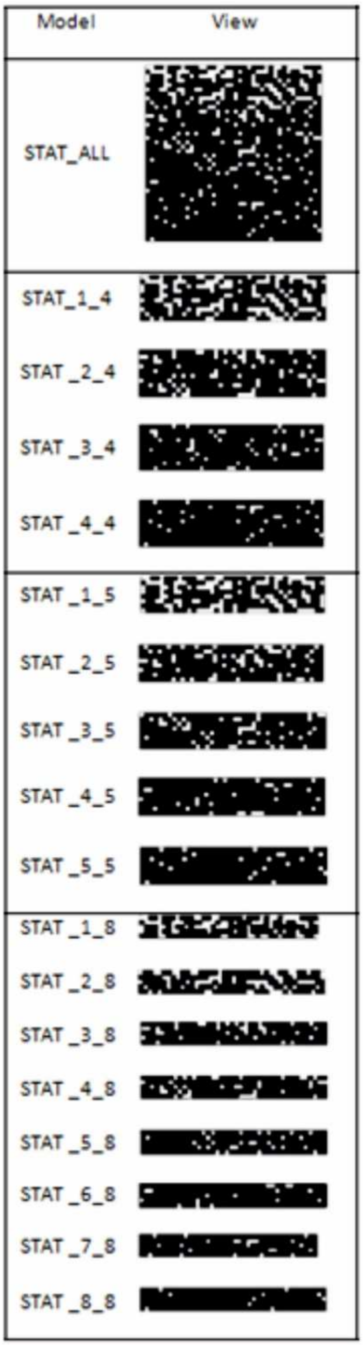

Fig. 6. Numerical models applied for homogenization method tests - models with normal distribution before homogenization

Rys. 6. Modele numeryczne użyte do testów metody homogenizacji - modele o rozkładzie normalnym przed homogenizacją

The behavior before compaction is orthotropic where the components of the stress tensor are uncoupled, i.e., an a component of strain will generate resistance in the local a-direction with no coupling to the local b and c directions. The elastic moduli vary from their initial values to fully compacted values at V_f, linearly with the relative volume V:

$$E_{aa} = E_{aau} + \beta(E - E_{aau}) \tag{1}$$

$$E_{bb} = E_{bbu} + \beta(E - E_{bbu}) \tag{2}$$

$$E_{cc} = E_{ccu} + \beta(E - E_{ccu}) \tag{3}$$

$$G_{ab} = E_{abu} + \beta(G - G_{abu}) \tag{4}$$

$$G_{bc} = E_{bcu} + \beta(G - G_{bcu}) \tag{5}$$

$$G_{ca} = E_{cau} + \beta(G - G_{cau}) \tag{6}$$

where

$$\beta = max\left[min\left(\frac{1-V}{1-V_f}, 1\right), 0\right] \tag{7}$$

and G is the elastic shear modulus for the fully compacted honeycomb material

$$G = \frac{E}{2(1+\nu)} \tag{8}$$

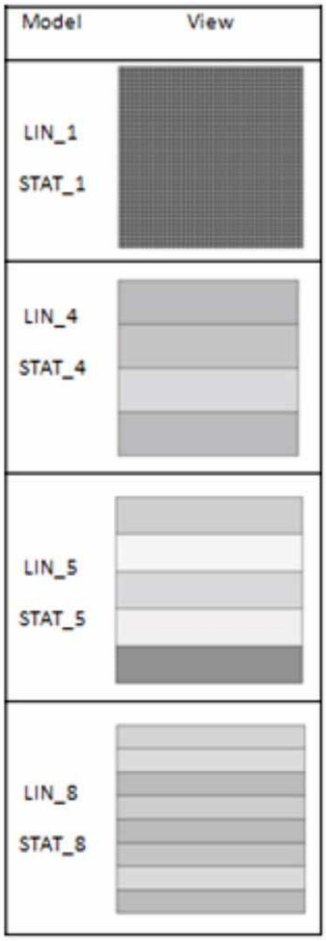

Fig. 7. Numerical models applied for homogenization method tests - after homogenization

Rys. 7. Modele numeryczne użyte do testów metody homogenizacji - po homogenizacji

The relative volume, V, is defined as the ratio of the current volume to the initial volume. Typically, $V = 1$ at the beginning of a calculation. The load curves define the magnitude of the average stress as the material changes density (relative volume) (see Fig. 8). There are two ways to define these curves, a) as a function of relative volume (V) or b) as a function of volumetric strain defined as:

$$\varepsilon_V = 1 - V \tag{9}$$

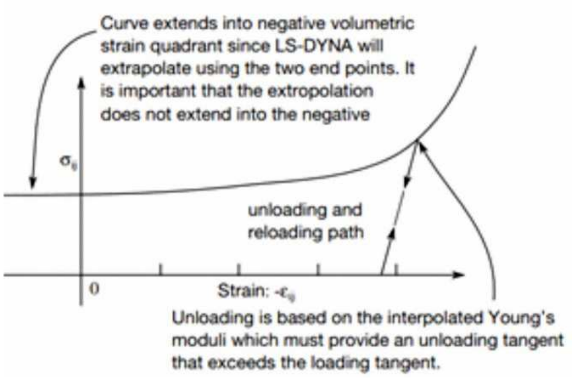

Fig. 8. Stress quantity versus volumetric strain for MAT_026_ HONEYCOMB material model

Rys. 8. Wartość naprężenia względem odkształcenia objętościowego dla modelu materiału MAT_026_HONEYCOMB

RESULTS AND DISCUSSION

The achieved results are presented in Tables 1 and 2 as errors of the homogenization method. The errors were calculated as a percentage difference between the FE analysis results for the model before and after homogenization.

TABLE 1. **Calculation results - percentage difference between results for model of linear distribution before and after homogenization**

TABELA 1. **Wyniki obliczeń - procentowa różnica między wynikami dla modelu o rozkładzie liniowym przed i po homogenizacji**

Model	Method error
LIN_ALL	40%
LIN_4	37%
LIN_5	18%
LIN_8	8%

TABLE 2. **Calculation results - percentage difference between results for model of normal distribution before and after homogenization**

TABELA 2. **Wyniki obliczeń - procentowa różnica między wynikami dla modelu o rozkładzie normalnym przed i po homogenizacji**

Model	Method error
STAT_ALL	44%
STAT_4	31%
STAT_5	20%
STAT_8	7%

CONCLUSIONS

Numerical tests of functionally graded composite homogenization were presented in the paper. On the basis of the obtained results, the method errors were calculated for each simulation. It is clearly visible that by applying thinner strips, a higher accuracy can be achieved. Unfortunately, the characteristic stress distribution around the grains and pores is always lost. The selection of strip thickness should be based on the required accuracy, accessible computational power and time of analysis. The disadvantage of such a kind of modeling is that assessment of the stress distribution in the microstructure is impossible.

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