PREDICTION OF THE EFFECTIVE YOUNG MODULUS OF 2D PERIODIC CELLS VIA FINITE ELEMENT ANALYSIS

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Abstract. *The macroscopic properties of composite materials depend on the microscopic properties of the constituents and the geometric arrangement of their phases. In this context, this research aims to predict material properties of a biphasic composite material composed of alumina inclusions surrounded by a glassy matrix using a bi-dimensional finite element model. Inclusions with the same diameter represent the disperse phase. In a first step, the dispersion algorithm allocates the particles randomly, allowing the overlapping between them, followed by a stepwise separation process up to a complete non-collision layout. Inclusions on the borders are mirrored or cut out to turn the cell periodic. A finite element model is used, with boundaries conditions applied over the element. The comparison between the numerical predictions and experimental data showed a maximum difference of 5.3 % for the temperature range without the presence of cracks. Improvements must be implemented concerning the periodic boundary conditions and new material models to simulate the matrix failure process.*

1. INTRODUCTION

Ceramic materials have broad use in high temperature applications, mainly as refractories materials. Drawbacks concerned with the microcracks generation related to stress fields restrict the usage of these materials. Microcracks arise at high temperatures gradients associated with different thermal expansion coefficients between the dispersed and continuous phases. Understanding this phenomenon is essential to develop new materials with better elastic properties. Many researchers have studied the drop in mechanical strength on composites materials due to damages related to temperature variation. Selsing (1961) [1] calculated the internal stress in biphasic materials considering spheres for the dispersed phase. Davidge and Green (1968) [2] proposed an analytical model that established a critical inclusion size depending on the thermomechanical properties and the thermal loading. According to their conclusions, beyond this critical size, microcracks would start to occur. Joliff et al. (2007) [3] studied the stress distribution between two inclusions to understand the interaction between the phases. In this context, this research aims to develop a numerical tool to predict the material properties of ceramic materials using finite element methods.

Elastic properties of heterogeneous materials measured by experimental means can take a lot of time and human labor due to the various possible configurations concerning these materials. With the development of finite element methods and an increase of the computational power, predictions via numerical methods have become a powerful tool to analyze the material properties of heterogeneous materials. The use of computational techniques to predict macroscopic properties of composite materials is possible due to homogenization methods. Homogenization is an averaging method applied to a volume element. The smallest volume of the material, which allows efficient computation of the macroscopic properties, is taken and represents statistically the material properties that can be used in macroscopic scales [4]. This volume is called Representative Volume Element (RVE). The difficulty in creating RVE to simulate composite materials is related to the geometric creation of the disperse phase. Microstructure generation depends on the material to be studied. Tessier-Doyen (2006) [5] used spherical inclusions composed of alumina immersed in a glassy matrix to study the elastic properties of composite materials. The present work focuses on the analysis of the same material investigated by them.

Among the various types of procedures available in the literature to create a dispersion of spheres of the same diameter (monodisperse spheres), the most intuitive and widely used is the random sequential adsorption method [6]. Still, it is not suitable for high volume fractions due to high computing time to insert new inclusions at high fractions (guaranteeing not overlapping between particles). References [7, 8] shows examples of this placement procedure used by some researchers to generate RVE. There are also the collective rearrangement algorithms that use an initial random distribution of particles, which allows overlapping followed by a separation process between the particles that will create a denser packing. The present research will deal with materials with a maximum 45% volume fraction as per [5], and the majority of methods are applicable. Still, the chosen one is the geometric generation by the collective rearrangement process, with a random overlapping process followed by a stepwise separation between the colliding particles.

2. MATERIALS AND METHODS

2.1. Numerical procedure

In Fig. 1 it is shown a chart describing the process of model generation since the input data, as the volume fraction and domain size, up to the plotting of the results. It illustrates how the data flows between the different software used. After having defined the number and position of the particles in the domain, it is necessary to turn it periodic. The periodic condition of the geometry of the RVE is necessary to represent the material correctly. Periodicity implies the repetition of the interior and borders of the geometry related to its left and right neighborhoods as well as with the upper and lower cell's neighbors [9]. Periodicity is the most challenging task related to geometry construction (compared with random dispersion and separation). Some circles suppress during this routine, others are cut out, and others are created by mirroring in such a way that the required volume fraction will be different from the initial defined. The insertion of new circles fulfills the difference between the expected and current volume fraction. New circles are placed randomly inside the domain in such a way that they do not overlap any existing sphere, and either does not cross the boundaries of the area.

2.2. Finite element model

In this research, the finite element model was created based on the experimental studies made by [5], where Tessier-Doyen and others studied the effect of the mismatch in the coefficient of thermal expansion (CTE) between the dispersed and matrix phases on the elastic properties of the ceramic composite material as the temperature varies. They used a ceramic composite material composed of alumina (Al_2O_3) inclusions immersed in glass bore-silicate matrix with volume fractions of 15%, 30%, and 45% for three different kinds of glass materials mixed with the disperse alumina phase to obtain three typical microstructure configurations ($\Delta\alpha < 0$, $\Delta\alpha = 0$ and $\Delta\alpha > 0$, where $\Delta\alpha$ denotes the CTE difference between matrix and inclusions). As damages are not expected to occur in the case with zero CTE, it has not been included in this research.

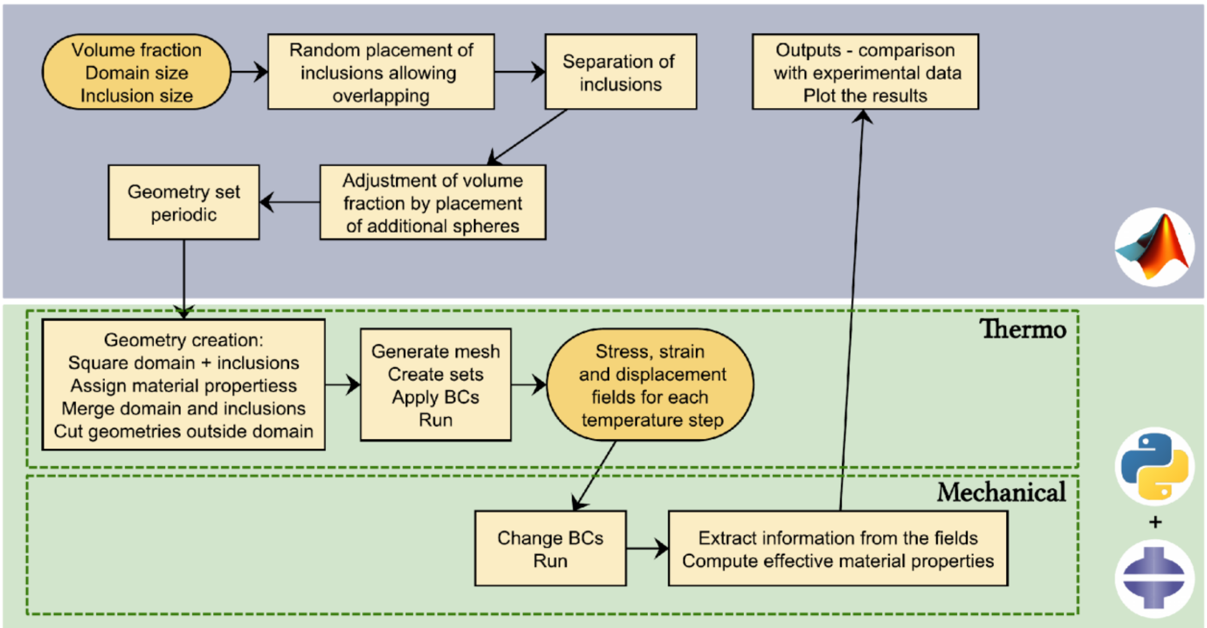
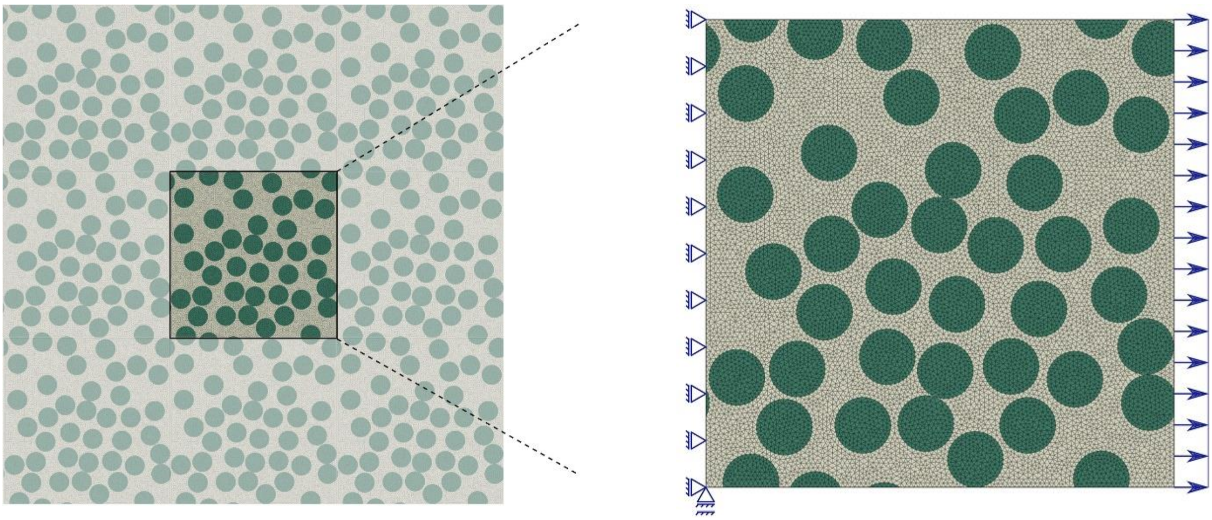


Figure 1 – Flowchart of the entire process

Figure 2a represents the RVE with the periodicity condition and Fig. 2b the boundaries conditions applied to the RVE for the mechanical analyses. The left face nodes have their horizontal displacement constrained (u = 0); the lower left vertex is pinned (u = 0, v = 0); and a prescribed displacement of u = 0.01 mm is imposed on the right face. The mesh was generated using triangles and quadrilateral linear finite elements. The properties used for alumina and glassy phases are summarized in Tab. 1.



(a) (b)

Figure 2 – RVE of the element and boundary conditions of the FEM

Table 1 – Material properties.

Material	Properties	T (°C)						
		25	**100**	**200**	**300**	**400**	**500**	**600**
Alumina	α (10^{-6} K^{-1})	4.8	5.3	6.2	6.8	6.8	7.1	7.4
	E (GPa)	340	335	330	325	320	315	310
	Poisson (ν)				0.24			
G1	α (10^{-6} K^{-1})	3	4.33	4.33	4.33	4.33	4.33	4.33
	E (GPa)				68			
	Poisson (ν)				0.20			
G3	α (10^{-6} K^{-1})	5.7	9.7	10.7	10.9	11.3	13.7	-
	E (GPa)	72	71	70	68	64	57	-
	Poisson (ν)				0.23			

2.3. Effective Young modulus computation

The Young modulus (E) calculation is based on Hooke´s law described as:

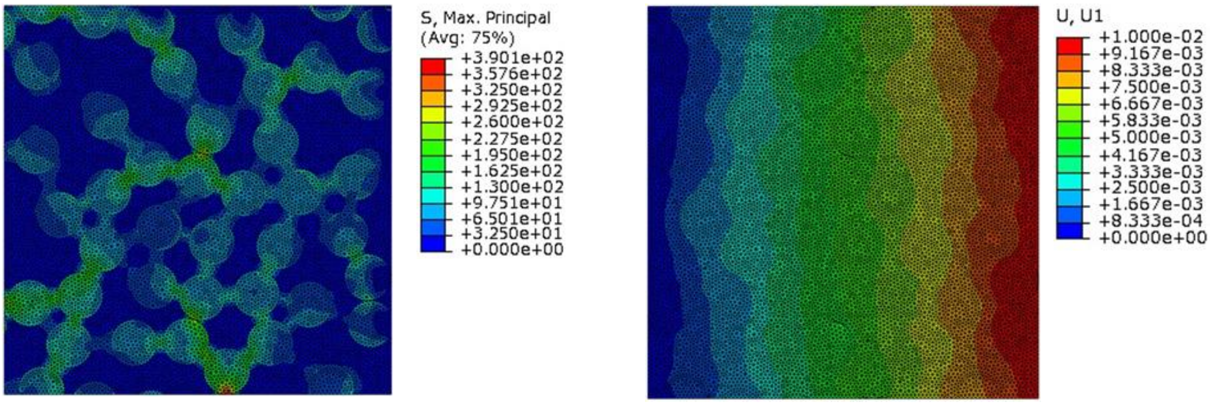
$$E = \sigma / \varepsilon \tag{1}$$

where ε is the deformation and σ the stress. For the finite element model used herein, the stress can be computed as the ratio between the sum of reaction forces and left face area. The macroscopic deformation ε is computed from the ratio between the prescribed displacement and the RVE side, i.e. $\varepsilon=u/L_0$. Virtual testings were performed at four different temperatures for each material. For the composite alumina/G1 the temperatures are: 25 ºC, 125 ºC, 277 ºC and 600 ºC. For alumina/G3: 25 ºC, 125 ºC, 277 ºC and 522 ºC. The results of the Young modulus were obtained through an average over five different geometrical samples that were compared with the experimental data.

3. RESULTS

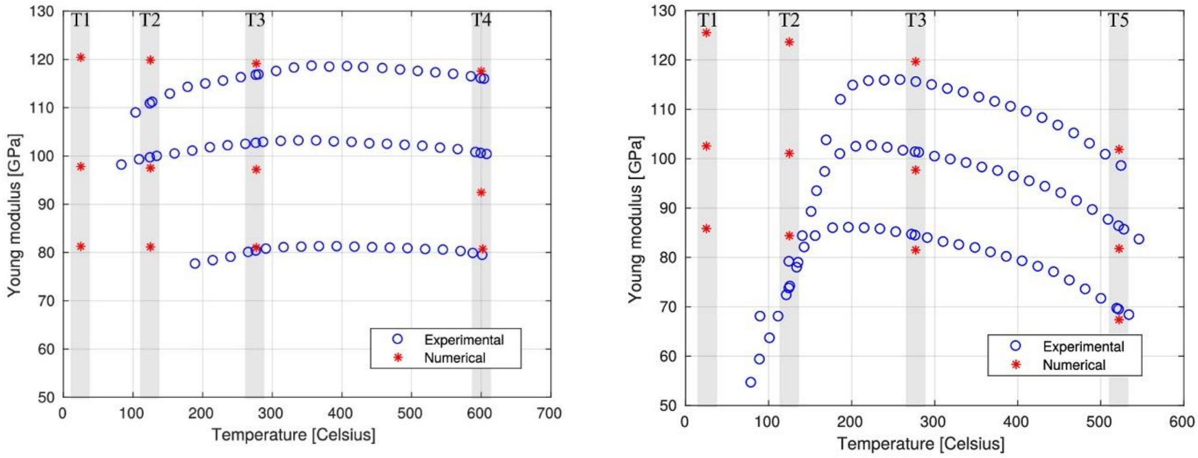
In Fig. 3, it can be seen the maximum principal stress field and the displacement concerning the material system alumina/G1. The stress field is shown in Fig. 3a for a temperature variation of 575 ºC. In Fig. 3b, the displacement shown is related to the mechanical phase for the temperature of 600ºC. The temperature variation led to internal stress due to the misfit between the thermal expansion coefficients. Since there are no periodic constraints imposed over domain boundary, there is not a continuity of the field of interest regarding left/right and bottom/top sides. The prescribed displacement in the right side results in a nonregular internal displacement field because of the randomness of dispersed arrangement.

In Fig. 4, it can be seen the differences between the experimental and numerical testings obtained through this work. The model predicts the values quite well from the higher temperatures (T4 and T5) down to temperatures a little lower than T3. Below this value, the CTE mismatch can induce the failure of the matrix/inclusion interface or cracks throughout the matrix, reducing the Young modulus considerably. This phenomenon becomes evident for the lower temperatures, which corresponds to more significant temperature variations. As the developed numerical model has no matrix failure model implemented, there was a significant difference in observed values for lower temperatures. Young modulus for T1 temperature cannot be compared due to inexistent experimental data.



(a) (b)

Figure 3 – Maximum stress and horizontal displacement field for an heterogeneous material with volume fraction of 45 vol. %



(a) Alumina / Glass 1 (b) Alumina / Glass 3

Figure 4 – Comparison between numerical predictions and experimental data obtained by Tessier-Doyen [5].

The difference between the experimental and numerical values are described in Tab. 2. For the material Alumina/G1, the values are compared for temperature T2 up to T4, and for Alumina/G3, for T2, T3 and T5 values. A maximum difference of 5.3% was obtained for the region without the presence of several cracks in the material. Regarding lower temperature variations, the maximum difference numerical/experiment was obtained for the Alumina/G1 30 vol. % material.

Table 2– Percentual difference between the predicted Young modulus with respect to the experimental values obtained by Tessier-Doyen [5].

	Material					
		Alumina/G1			**Alumina/G3**	
Volume fraction	**15%**	**30%**	**45%**	**15%**	**30%**	**45%**
T1 (25 ºC)	-	-	-	-	-	-
T2 (125 ºC)	-	2	8.2	1.5	27	67
T3 (277 ºC)	0.9	5.3	2.1	3.4	3.6	3.6
T4 (600 ºC)	1.7	4	1.3	-	-	-
T5 (522 ºC)	-	-	-	2.9	5.2	3.4

4. CONCLUSION

In the present article, a computational tool to predict the effective properties of heterogeneous materials based on numerical simulations using the finite element method was presented. The algorithm developed enabled to simulate several bidimensional arrangements with a random particle distribuition. The effective properties identified for alumina/glass composites have shown to agree with the experimental data of the literature, with a difference inferior to 5.3% for temperatures without the evidence of cracks. The next features of the computational tools concern the application of periodic boundary conditions for non-matching meshes and the implementation of three-dimensional models.

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