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Effective elastic properties of alumina-zirconia composite ceramics by a 2D computational homogenization procedure

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Abstract. Composites have applications in many industrial segments, where different materials are combined to obtain improved mechanical properties. Thus, the determination of the macroscopic constitutive behavior of composites with accuracy is important to provide the desired properties. In this context, the present work explores a 2D computational homogenization procedure to compute the effective elastic properties of alumina-zirconia composite ceramics. The average-based homogenization theory is used to obtain the homogenized or effective constitutive behavior. The composite is modeled by the concept of Representative Volume Element (RVE), which is numerically simulated with finite elements. Simulations are performed considering the uniform and periodic boundary conditions. The computationally homogenized results for the elasticity modulus are close to the experimental results compared. The boundary condition has a significant influence in the case of the shear modulus. Furthermore, the computational homogenization framework is an interesting tool for designing composites with specific properties.

Keywords. composite ceramics, effective elastic properties, computational homogenization, finite elements, uniform and periodic boundary conditions

1 Introduction

Alumina-zirconia (AZ) composites have a wide range of applications [1–3]. This composite material combines the high hardness of alumina and the excellent fracture resistance of zirconia [1]. Furthermore, its widespread use is due to a combination of good strength, moderate fracture toughness, high wear resistance, good biocompatibility and excellent corrosion resistance [3]. In this context, alumina-zirconia composites are attractive structural materials [3, 4]. On the other hand, obtaining the desired macroscopic properties of a composite requires a sufficiently precise knowledge of its effective constitutive behavior.

The effective elastic properties can be of particular interest in many applications. In this sense, different strategies were developed to estimate the effective or macroscopic constitutive behavior of composites. The rule of mixtures proposed by Voigt (upper bound) and Reuss (lower bound) are well-known models for estimating effective properties [5, 6]. Another well-known estimates are the Hashin–Shtrikman bounds considering the use of minimum potential energy and minimum complementary energy principles [7]. Over time, other strategies have also been explored to estimate effective properties more accurately.

In particular, computational homogenization strategies have been used successfully to predict the effective constitutive behavior of heterogeneous media. For example, some recent works presented computational homogenization tools to study the effective constitutive behavior of composites and porous media using the ABAQUS® software [8, 9]. In this context, the present work

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explores a two-dimensional computational homogenization procedure to compute the effective elastic properties of alumina-zirconia composite ceramics. The tool for computational homogenization was implemented in ANSYS® Mechanical, Release 18.0. The composite is modeled with the concept of RVE formed by a circular zirconia inclusion inserted in the alumina matrix. Two boundary conditions are imposed on the RVE: (i) homogeneous strain boundary condition; (ii) periodic boundary condition. The effective elastic properties by computational homogenization are compared with experimental data and the theoretical formulation proposed in the literature [10]. Finally, approximate closed expressions are obtained to estimate the elastic parameters based on the volume fraction of zirconia inclusion.

2 Basic concepts of the average-based homogenization theory

In the context of average-based homogenization theory, the macroscopic strain (E) and stress (Σ) tensors can be obtained based on the volume averaging of the microscopic strain (ε) and stress (Σ) tensors over a RVE [11]:

$$E =< \varepsilon >= \frac{1}{V} \int_V \varepsilon dV \tag{1}$$

$$\Sigma =< \sigma >= \frac{1}{V} \int_V \sigma dV \tag{2}$$

where $< \cdot >$ indicates the volume average of the microscopic fields over the RVE; and V is the total initial volume of the RVE.

The Hill and Mandel principle [11, 12] allows the association of macro-micro scales by energy equivalence :

$$\Sigma : E = \frac{1}{V} \int_V \sigma : \varepsilon dV =< \sigma : \varepsilon > \tag{3}$$

The homogenized stress and strain tensors (Σ and E) can be correlated through the constitutive law. One option is to use Hooke's Law considering the effective elastic stiffness tensor ($\mathbb{C}_{ef}$):

$$\Sigma = \mathbb{C}_{ef} : E \tag{4}$$

In addition, another option is to use Hooke's Law considering the effective elastic flexibility tensor ($\mathbb{D}_{ef}$):

$$E = \mathbb{D}_{ef} : \Sigma \tag{5}$$

where $\mathbb{D}_{ef} = (\mathbb{C}_{ef})^{-1}$.

The macroscopic constitutive behavior requires the solution of a Boundary Value Problem (BVP) for the RVE. In this sense, two well-known boundary conditions in the literature are: (i) uniform strain boundary condition (USBC); and (ii) the periodic boundary condition (PBC).

The uniform strain boundary condition (USBC) is given by:

$$u = E^* \cdot x \quad \forall \quad x \in \partial V \tag{6}$$

where E^* is the macroscopic homogeneous strain tensor imposed on the RVE boundary; u is the displacement field; and x is the position vector. In this case, after some deductions, we can prove that $E =< \varepsilon >= E^*$.

The periodic boundary condition (PBC) is given by:

$$u = E^* \cdot x + \tilde{u} \quad \forall \quad x \in \partial V \tag{7}$$

where $\tilde{u}$ is called periodic fluctuation. After some deductions, we can also prove that $E =< \varepsilon >= E^*$. Moreover, note that $< \tilde{u}_{i,j} >= 0$ when volume averaging process is performed over the RVE.

3 Effective properties by a 2D computational homogenization procedure

In this work, a 2D computational homogenization procedure is explored to determine the effective elastic properties of alumina-zirconia composite ceramics. Initially, the material properties and RVE mesh must be defined. Afterward, the Boundary Value Problem is solved with numerical simulations by the Finite Element Method. Finally, the macroscopic fields are obtained based on the volume averaging of the microscopic fields computed with finite element simulations. In this context, the main data to simulate the composite as well as the details of the computational homogenization procedure are presented below.

3.1 RVEs: elastic properties and meshes

The effective elastic properties of alumina-zirconia composite ceramics (AZ composites) are investigated in this work. The properties of the constituents were adopted from the theoretical/experimental study presented by Pabst et al. [10]. Table 1 presents the values for the elasticity modulus (Y), the shear modulus (G) and the compressibility modulus (K). It is worth mentioning that the Poisson coefficients of each constituent material can be obtained by conventional linear elasticity relationships based on known elastic parameters. Thus, the Poisson coefficients for matrix and inclusion are $\nu_m = 0.23$ and $\nu_i = 0.31$, respectively.

Table 1: Properties of constituents [7].

Material	Y (GPa)	G (GPa)	K (GPa)
Alumina matrix	$400 \pm 2\%$	$163 \pm 1\%$	$247 \pm 1\%$
Zirconia inclusion	$210 \pm 4\%$	$80 \pm 2\%$	$184 \pm 2\%$

The effective elastic properties were obtained for the following inclusion volume fractions (f): 0.05; 0.1; 0.2; 0.3; 0.4; 0.5 and 0.6. The mesh for each case is shown in Figure 1. The 6-node triangular element was used in the numerical simulations with the FEM.

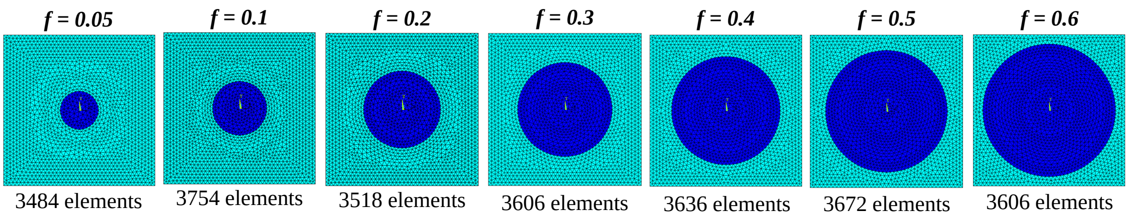

Figure 1: Meshes for seven values of inclusion volume fraction (f).

3.2 Computational homogenization procedure

The computational homogenization framework was implemented in ANSYS® Mechanical, Release 18.0. After numerical simulations with finite elements considering USBC or PBC, the homogenized stress tensor (Σ) can be computationally obtained by the following expression:

$$\Sigma = < \sigma > = \frac{1}{V} \sum_{i=1}^{N_{elem}} \sigma_i V_i \tag{8}$$

where N_{elem} is the number of finite elements; σ_i is the average stress in the element i computed from the integration points; V_i is the element volume i; and V is the total initial volume of the RVE. Furthermore, the homogenized strain tensor is given by the macroscopic homogeneous strain tensor imposed on the RVE boundary ($E = E^*$).

The results are obtained from two-dimensional analysis. Considering the components of the two-dimensional case and the symmetry of the stress and strain tensors, the constitutive law can be written in a simplified way as:

$$\left\{ \begin{array}{c} \Sigma_{11} \\ \Sigma_{22} \\ \Sigma_{12} \end{array} \right\} = \left[\begin{array}{ccc} C_{1111} & C_{1122} & C_{1112} \\ C_{1122} & C_{2222} & C_{2212} \\ C_{1112} & C_{2212} & C_{1212} \end{array} \right] \left\{ \begin{array}{c} E_{11} \\ E_{22} \\ 2E_{12} \end{array} \right\} \tag{9}$$

The effective components of $\mathbb{C}_{ef}$ are determined from the homogenized fields of Σ and E. Thus, values of E^* must be conveniently imposed to obtain the components of $\mathbb{C}_{ef}$. In this case, we performed the following analyses considering normal and shear acroscopic strains: (i) $E^*_{11} = 1.0$; (ii) $E^*_{22} = 1.0$; and (iii) (i) $2E^*_{12} = 1.0$. Finally, the homogenized elastic properties (Y_{ef}, G_{ef} and ν_{ef}) can be determined from $\mathbb{C}_{ef}$.

4 Results and discussion

The effective elastic properties are shown in Figure 2. The results are compared with experimental data and the theoretical formulation extracted from Pabst et al. [10]. Moreover, the upper bound of Voigt (or iso-strain assumption) and the lower bound of Reuss (or iso-stress assumption) are also presented for Y_{ef} and G_{ef}. It should be noted that it is not suitable to calculate the Poisson's ratio under the iso-strain and iso-stress assumptions. Thus, the results for the the rule of mixtures[5, 6] are not shown for ν_{ef}.

The results of Y_{ef} by computational homogenization are in good agreement with experimental data and the theoretical formulation extracted from Pabst et al. [10]. In addition, the computationally homogenized results are between upper and lower limits of Voigt and Reuss, respectively. In this case, the boundary condition has no significant influence on the homogenized results. It is worth mentioning that the distribution of microscopic fields is important to understand the macroscopic or effective results. The distributions of microscopic normal stress are close for USBC and PBC. Therefore, the effective results of the modulus of elasticity are close for both boundary conditions.

In the case of G_{ef}, only the effective responses with USBC are close to the theoretical formulation proposed by Pabst et al. [10]. On the other hand, effective results with PBC clearly represent a lower bound when compared to USBC. Therefore, the boundary condition has a significant influence on the macroscopic results. This difference in the effective shear modulus is correlated with the distribution of microscopic fields. As shown in Figure 3, the distribution of microscopic shear stresses with USBC has strong differences when compared to PBC. Finally, the results considering ν_{ef} are close for both USBC and PBC. Furthermore, there are differences between the computationally homogenized results and the theoretical formulation proposed by Pabst et al. [10]. Despite these visible differences, the results compared are in good agreement.

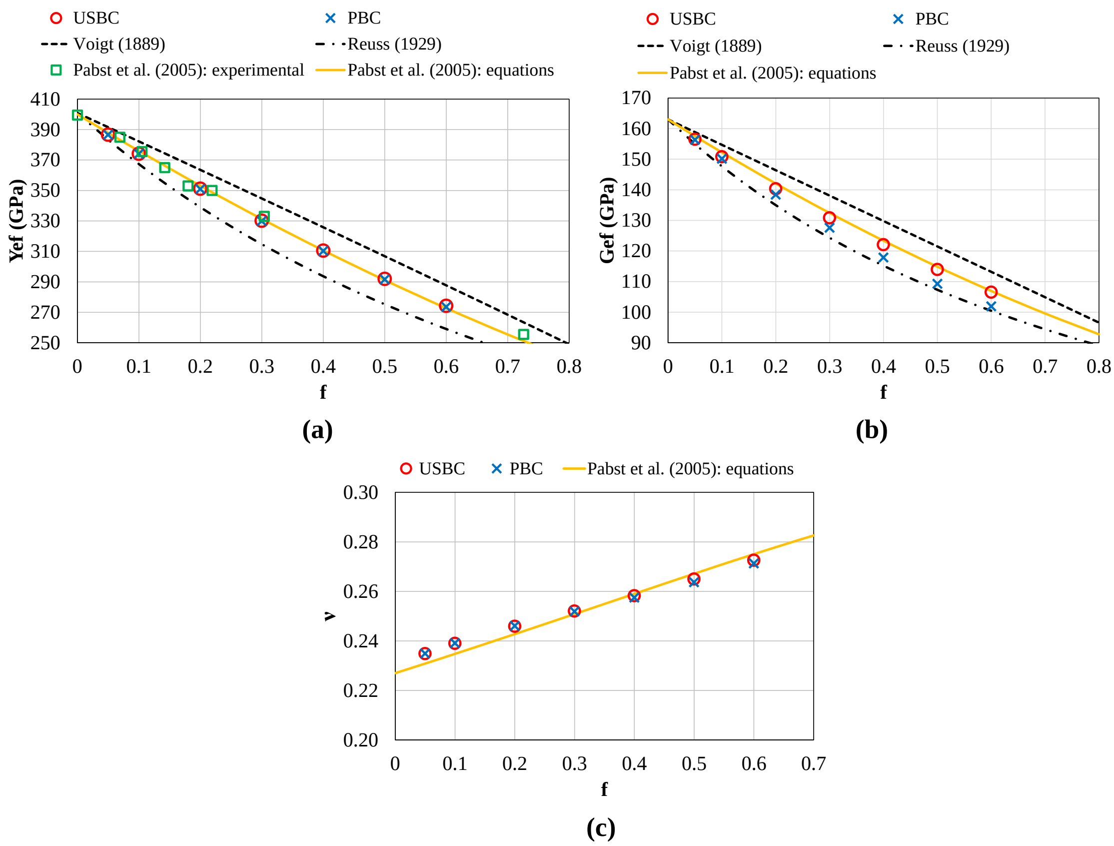

Figure 2: Effective elastic properties.

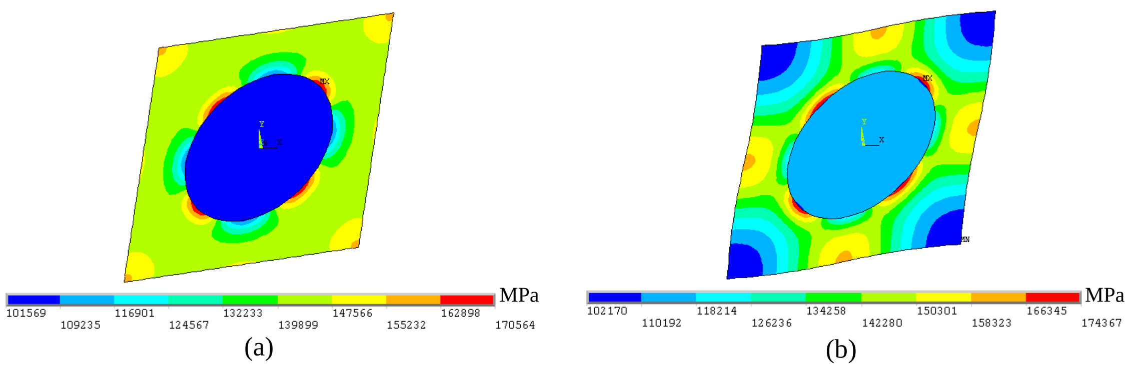

Figure 3: Microscopic shear stresses σ_{12} for the RVE with $f = 0.3$ under $2E^*_{12} = 1.0$: (a) USBC; (b) PBC.

Figure 4 shows closed approximate expressions to estimate the effective elastic properties as a function of f (inclusion volume fraction). Note that polynomial expressions were used to approximate the results for USBC and PBC. The value of $R^2 \approx 1$ indicates a good agreement between the approximate expressions and the numerical results.

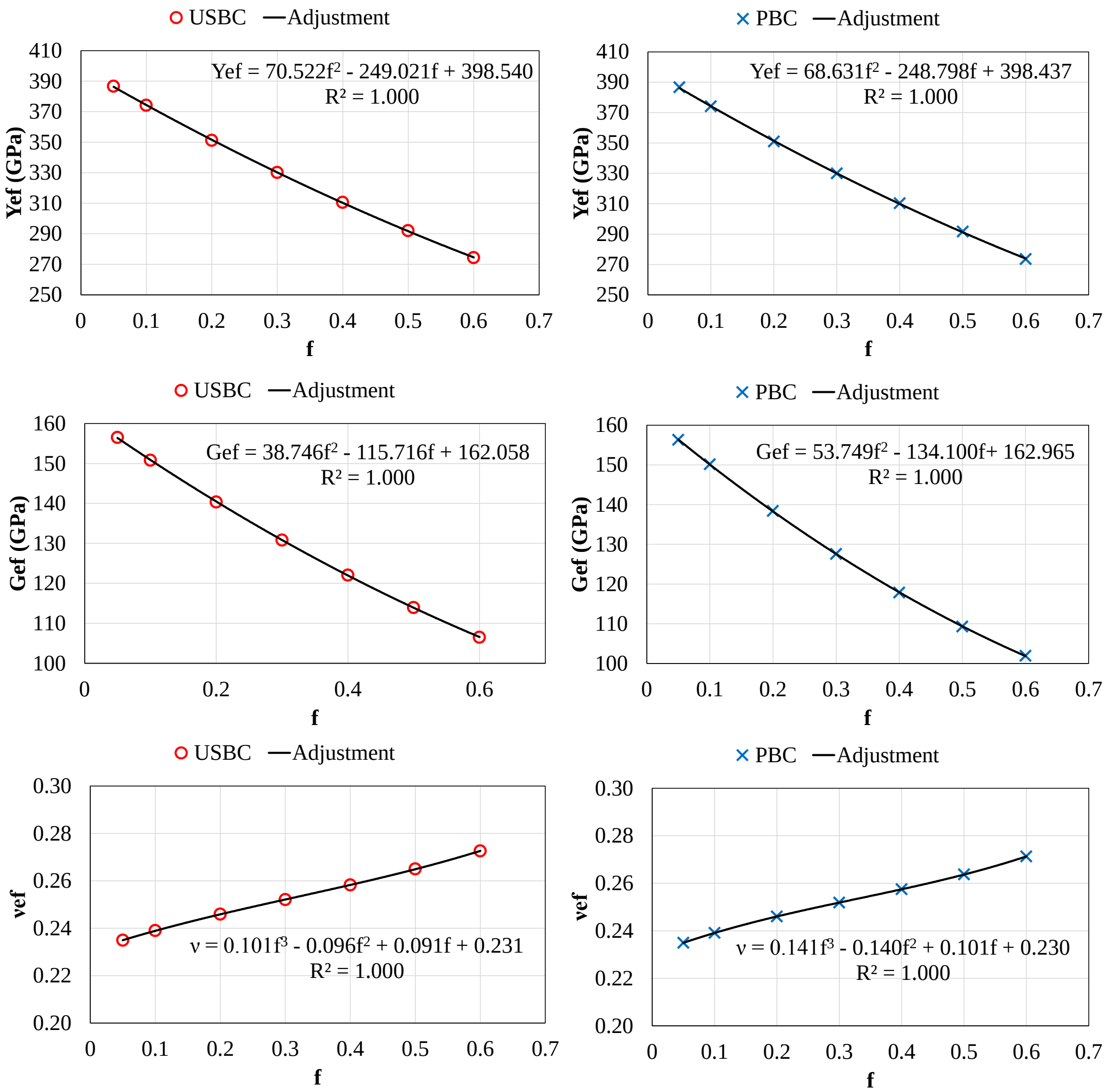

Figure 4: Approximate functions for Y_{ef}, G_{ef} and ν_{ef} considering USBC and PBC.

The approximate expressions considering USBC are:

$$Y_{ef} = 70.522f^2 - 249.021f + 398.540 \quad (10)$$

$$G_{ef} = 38.746f^2 - 115.716f + 162.058 \quad (11)$$

$$\nu_{ef} = 0.101f^3 - 0.096f^2 + 0.091f + 0.231 \quad (12)$$

The approximate expressions considering PBC are:

$$Y_{ef} = 68.631f^2 - 248.798f + 398.437 \quad (13)$$

$$G_{ef} = 53.749f^2 - 134.100f + 162.965 \quad (14)$$

$$\nu_{ef} = 0.141f^3 - 0.140f^2 + 0.101f + 0.230 \quad (15)$$

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5 Conclusions

In this work, a 2D computational homogenization procedure was explored to obtain the effective elastic properties of alumina-zirconia composite ceramics. In general, the numerical responses showed good agreement with the compared reference results. The results of the effective properties from USBC and PBC are close for the modulus of elasticity and Poisson's coefficient. In the case of the shear modulus, only the effective responses with USBC are close to the compared reference result. Thus, the boundary condition has a significant influence on the shear modulus, where USBC provides an upper limit when compared to PBC. It is worth mentioning that closed approximate expressions were also proposed to estimate the effective elastic properties based on the inclusion volume fraction. Furthermore, this computational approach allows modeling changes in morphology, elastic properties and volume fractions of the constituents. Therefore, the computational homogenization procedure explored in this work can be an interesting tool in the development/design of heterogeneous materials with improved mechanical properties.

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