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Numerical estimation of effective mechanical properties in polycrystalline materials from a microscale analysis using the Boundary Element Method

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Abstract. In this paper, the effective mechanical properties of polycrystalline materials are determined from a microscale analysis using the Boundary Element Method. The macroscopic behavior of polycrystalline materials, such as ceramics and metals, is directly related to their microstructure. Therefore, it is of interest to determine the apparent mechanical properties of the material, based on its heterogeneous behavior at the microscale. These materials have a microstructure composed of several grains, with different orientations and, consequently, different mechanical properties. For this reason, a multiregion formulation of the Boundary Element Method is used in the analysis of polycrystalline microstructures, in which each grain is treated as a domain with orthotropic behavior and random crystallographic orientation. The formulation is based on the displacement boundary integral equation, with the use of anisotropic fundamental solutions, so that the entire problem is written in terms of the displacements and tractions measured at the grain boundaries. The integrity of the polycrystalline aggregate is ensured by imposing interface conditions that guarantee the equilibrium of tractions and prevent relative displacements between the faces of two adjacent grains. The artificial morphology of the polycrystalline aggregate is generated using Voronoi tesselations. The described formulation is applied to the analysis of polycrystalline aggregates in order to determine their effective mechanical properties.

Keywords: Effective isotropic properties, Polycrystalline microstructure, Multiregions, Boundary Element Method

1 Introduction

Although polycrystalline materials, such as ceramics and metals, are considered homogeneous at the macroscopic level, they exhibit heterogeneous behavior at the microstructural level, since their microstructure is composed of several grains with distinct material properties and random crystallographic orientation. From the heterogeneous behavior of the material at the microscale, the effective properties of the homogeneous macrocontinuum, such as elastic modulus and Poisson ratio, can then be determined. In this context, a multiregion formulation of the Boundary Element Method presents itself as a robust tool, since the problem is written in terms of grain boundary variables only, such as displacements and tractions, reducing the computational cost of the analysis.

The determination of apparent macroscopic properties of metals and ceramics, based on the study of the material behavior at the microscale using a multiregion formulation of the Boundary Element Method, has been the focus of several studies in the literature. Sfantos and Aliabadi [1] and Benedetti and Aliabadi [2] determined the macroscopic effective properties of SiC, as well as studied the nucleation and propagation of microcracks in polycrystalline aggregates of the same material. Benedetti and Aliabadi [3] estimated the mechanical properties of FCC metals, such as copper, gold and nickel. Gulizzi et al. [4] evaluated the apparent properties of copper, SiC and a two-phase stainless steel SAF2507, in terms of effective elastic and shear moduli. Galvis et al. [5] determined elastic properties, such as elastic modulus, shear modulus and the stiffness tensor of copper and zinc. Benedetti et al. [6] applied the formulation to determine the apparent properties of $BaTiO_3$ ceramics. More recently, Benedetti [7] performed the computational homogenization of SiC and Al_2O_3 ceramics under thermoelastic conditions.

In this paper, a multiregion formulation of the Boundary Element Method is employed to analyze two-dimensional SiC and Al_2O_3 microstructures in order to determine their effective elastic moduli and Poisson ratios. Considerations regarding the morphology and the material of the polycrystalline aggregate are presented in section 2, the BEM formulation is given in section 3, the numerical simulations and their results are detailed in section 4 and concluding remarks are given in section 5.

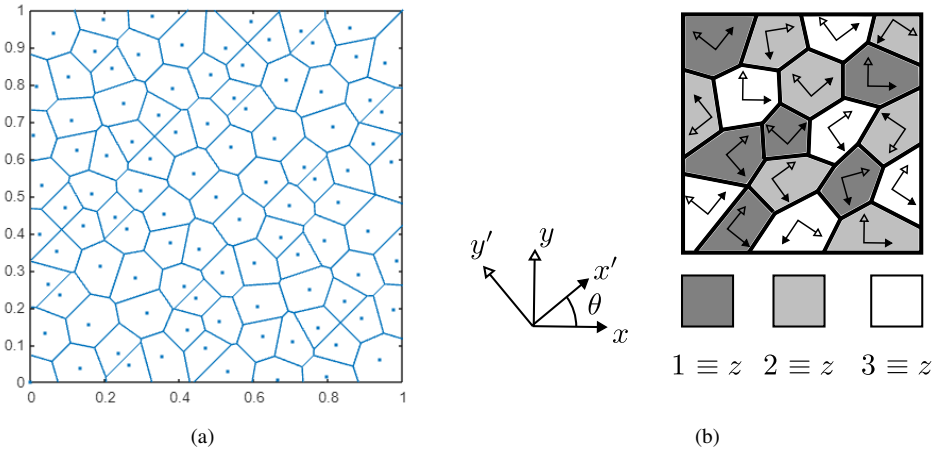
2 Artificial morphology and material considerations

Polycrystalline materials are represented by a microstructure composed of several grains. According to Van Vlack [8], the orientation of these grains within the microstructure is random and their shape is typically controlled by the presence of adjacent grains. To represent the microstructure of the analyzed ceramics, a Voronoi tesselation is used, constructed from initial points generated with the Sobol sequence. Figure 1(a) illustrates one of the microstructures to be analyzed, composed of 100 grains. After defining the artificial morphology, it is necessary to determine the properties of the analyzed polycrystalline material. In this work, each grain is considered orthotropic, with distinct elastic properties along three axes orthogonal to each other. According to Sfantos and Aliabadi [1] and Benedetti and Aliabadi [2], the consideration of orthotropy is appropriate, since most single ceramic and metallic crystals exhibit orthotropic behavior. Thus, the constitutive relations combining stresses and strains are given by:

$$\sigma_{ij} = c_{ijkl}\varepsilon_{kl}, \tag{1}$$

where σ_{ij} and ε_{kl} refer to the components of the stress and strain tensors, respectively, and c_{ijkl} denotes the components of the orthotropic stiffness tensor. For the orthotropic case, this stiffness tensor has only 9 non-zero constants, namely c_{1111}, c_{2222}, c_{3333}, c_{1122}, c_{1133}, c_{2233}, c_{1212}, c_{1313} e c_{2323}.

In this work, the behavior of grains within the polycrystalline aggregate is analyzed using a two-dimensional formulation. To capture the three-dimensional effect in a two-dimensional model, some assumptions were made. The first assumption concerns the adopted plane state. The analyses are performed considering plane strain, allowing the two-dimensional model to represent the three-dimensional effect by assuming that the out-of-plane dimension is sufficiently large. The second assumption adopted to capture the three-dimensional effect in the two-dimensional model concerns the different choices of the material axis coinciding with the z axis. The material coordinate system is defined as 123, while the geometric coordinate system is identified by xyz. Therefore, the microscale is considered to be in the xy-plane and, according to Espinosa and Zavattieri [9], to maintain deformations in this plane, one of the principal axes of the material must coincide with the z-axis. Three cases are considered: Case 1: $1 \equiv z$, Case 2: $2 \equiv z$ and Case 3: $3 \equiv z$. Furthermore, the local x' and y' axes are defined from a counterclockwise rotation by an angle θ from the global x and y axes. The material axis coinciding with the z-axis and the angle θ are defined randomly for each grain, as illustrated in Fig. 1(b), in order to mantain the stochastic effects and the random character of the microstruture.



(a) (b)

Figure 1. (a) Artificial morphology and (b) material orientation for polycrystalline media

3 Multiregion formulation of the Boundary Element Method

The analysis of the polycrystalline microscale is performed using a multiregion formulation of the Boundary Element Method, in which each grain is treated as a domain with specific material behavior and random crystallographic orientation. The boundaries of these grains are divided into contact, Γ_c, and non-contact boundaries,

Γ_{nc}, according to Fig. 2. At the non-contact boundary Γ_{nc}, coinciding with the microscale boundary, boundary conditions are imposed such that only one of the variables, displacement or tractions, is unknown. Meanwhile, the contact boundary, Γ_c, refers to the part of the grain boundary that is in contact with other grains boundaries. At Γ_c, both variables are unknown and interface conditions are imposed, which relate the displacements and tractions of adjacent grains. To ensure the integrity of the microscale, the relative displacement at the interface between two grains must be zero, and the equilibrium of tractions must be met. Therefore, considering two adjacent grains A and B, the following interface conditions are imposed:

$$\delta\tilde{u}_i^I = \tilde{u}_i^A + \tilde{u}_i^B = 0, \qquad \tilde{t}_i^I = \tilde{t}_i^A = \tilde{t}_i^B, \tag{2}$$

where $\delta\tilde{u}_i^I$ and $\tilde{t}_i^I$ represent the relative displacement and the traction of the interface and $\tilde{u}_i^A$, $\tilde{u}_i^B$, $\tilde{t}_i^A$ and $\tilde{t}_i^B$ are the displacements and tractions of grains A and B, respectively. In this equation, $(\tilde{\cdot})$ indicates that these variables are written in the local coordinates of the grain boundary, with i designating the normal and tangential directions.

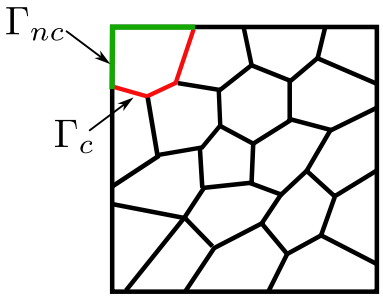


Figure 2. Contact and non-contact boundaries

As indicated in section 2, each grain has a random material orientation defined by an angle θ. When the reference coordinate system does not coincide with the material coordinate system, orthotropic grains exhibit apparently anisotropic behavior. In order to allow the use of anisotropic fundamental solutions simplified for the orthotropic case and to avoid the rotation of the fourth-order tensor presented in eq. (1), the functional grain boundary technique, proposed by Sfantos and Aliabadi [1], is used. This functional grain boundary is obtained by expressing the grain boundary coordinates in the material reference system, as Fig. 3.

The displacement Boundary Integral Equation is then solved for the functional grain boundary $\tilde{\Gamma}$:

$$\begin{aligned} c_{ij}(\boldsymbol{\xi})\tilde{u}_j(\boldsymbol{\xi}) + \fint_{\tilde{\Gamma}_{nc}} \tilde{t}_{ij}^*(\boldsymbol{\xi},\boldsymbol{x})\tilde{u}_j(\boldsymbol{x})\mathrm{d}\tilde{\Gamma}_{nc} + \fint_{\tilde{\Gamma}_c} \tilde{t}_{ij}^*(\boldsymbol{\xi},\boldsymbol{x})\tilde{u}_j(\boldsymbol{x})\mathrm{d}\tilde{\Gamma}_c = \int_{\tilde{\Gamma}_{nc}} \tilde{u}_{ij}^*(\boldsymbol{\xi},\boldsymbol{x})\tilde{t}_j(\boldsymbol{x})\mathrm{d}\tilde{\Gamma}_{nc} \\ + \int_{\tilde{\Gamma}_c} \tilde{u}_{ij}^*(\boldsymbol{\xi},\boldsymbol{x})\tilde{t}_j(\boldsymbol{x})\mathrm{d}\tilde{\Gamma}_c \end{aligned} \tag{3}$$

where $\boldsymbol{\xi}$ and $\boldsymbol{x}$ refer to the source and field points, respectively, $\tilde{u}_j$ and $\tilde{t}_j$ are the displacement and traction components in local coordinates, c_{ij} is the free term, which, on smooth surfaces, is given by $c_{ij} = \delta_{ij}/2$ and $\tilde{u}_{ij}^*$ and $\tilde{t}_{ij}^*$ are terms of the anisotropic fundamental solution, presented by Cruse and Swedlow [10], written in the local coordinates of the functional grain boundary, with i and j referring to the normal and tangential directions.

4 Numerical simulations

The formulation described is applied to determine the apparent properties of polycrystalline aggregates of silicon carbide (SiC) and alumina (Al_2O_3). The elastic constants adopted for each material are in Table 1.

To determine the effective properties, different microstructures are tested under simple traction conditions. Normal displacements on the left and bottom sides are restricted, while a uniform traction of $\sigma = 100$ MPa is applied to the right side. Figure 4 illustrates the imposed boundary conditions on a microstructure composed of 100 grains.

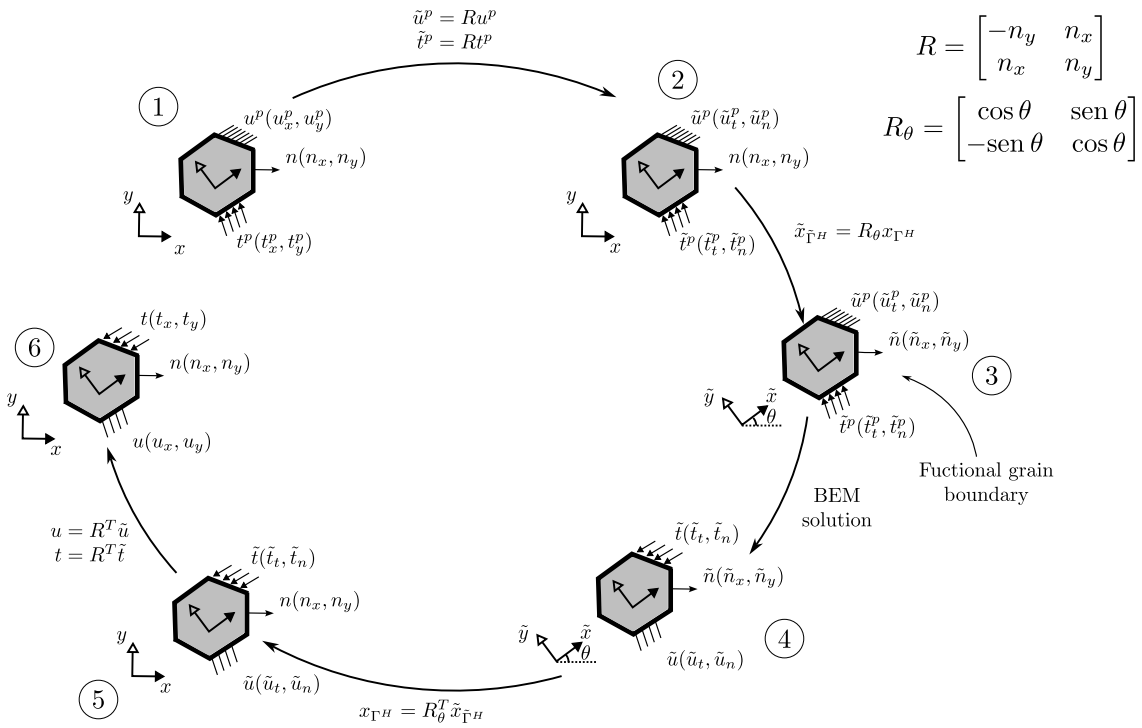


Figure 3. Solution procedure using functional grain boundary

Table 1. Elastic constants of SiC and Al_2O_3 polycrystalline aggregates (GPa)

	SiC	Al_2O_3
c_{1111}, c_{2222}	502	496.8
c_{3333}	565	498.1
c_{1122}	95	163.6
c_{1133}, c_{2233}	96	110.9
c_{2323}, c_{1313}	169	147.4
c_{1212}	203.5	166.6

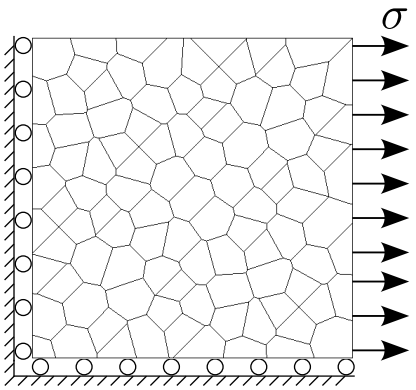


Figure 4. Schematic view of the microstructure boundary conditions

Since the numerical simulations are performed considering plane strain to represent the three-dimensional

behavior of the grains within the microstruture and knowing that $\sigma_{11} = \sigma$ and $\sigma_{22} = \sigma_{12} = 0$, the effective elastic modulus and Poisson ratio are determined by the following isotropic constitutive relations:

$$\varepsilon_{11} = \frac{(1-\nu^2)\sigma_{11}}{E} = \frac{(1-\nu^2)\sigma}{E} \tag{4}$$

$$\varepsilon_{22} = \frac{-\nu(1+\nu)\sigma_{11}}{E} = \frac{-\nu(1+\nu)\sigma}{E} \tag{5}$$

where ε_{11}, ε_{22}, σ_{11} and σ_{22} are components of the strain and stress tensors, respectively, σ is the applied load, E is the apparent modulus of elasticity, and ν is the effective Poisson ratio.

In order to evaluate the influence of the number of grains on determining effective properties, numerical simulations are performed for microstructures composed of 16, 20, 26, 32, 50, 70, 100, 150, 200 and 250 grains. Each microstructure is analyzed 50 times, varying the material axis coinciding with the z-axis and the angle θ. In each analysis, the elastic modulus and Poisson ratio are measured by eq. (4) and eq. (5), and the results are presented in terms of the scatter, mean values and the standard deviation for each microstructure. Figure 5 illustrates the results for silicon carbide, while, for alumina, the results are presented in Fig. 6.

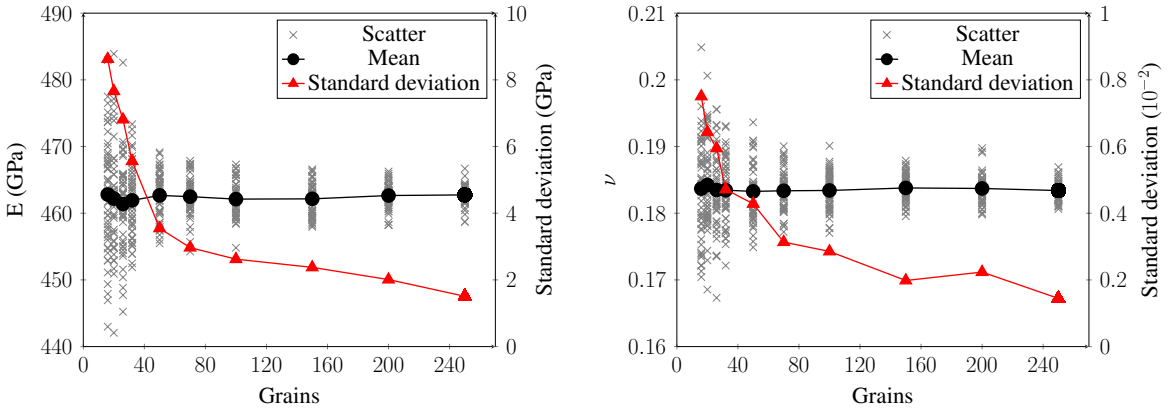


Figure 5. Effective properties of silicon carbide, being (a) elastic modulus and (b) Poisson ratio

As illustrated in Fig. 5(a), the mean elastic modulus for each microstruture ranges from 461 GPa to 463 GPa, with a mean value of 462.3 GPa across all simulations. These values are in good agreement with those reported in the literature, since Benedetti and Aliabadi [2] reported a mean value of 456 GPa, Sfantos and Aliabadi [1], a mean value of 468 GPa, Kubler [11] reported E = 460 GPa and Hertzberg [12], E = 470 GPa. For the effective Poisson ratio, presented in Fig. 5(b), the mean values ranged from 0.1832 to 0.1845, with an average of 0.1836, within the range expected by Shackelford and Alexander [13], which ranges from 0.183 to 0.192.

According to Fig. 6(a), the mean values for the alumina apparent elastic modulus varied between 405 GPa and 409 GPa, with an average of 407.2 GPa, considering all simulations. Meanwhile, the effective Poisson ratio (Fig. 6(b)) was between 0.2345 and 0.2368, with a mean value equal to 0.2359. These values are in good agreement with the literature, since Yousef et al. [14] report values between 375 GPa and 400 GPa for the alumina elastic modulus, while Benedetti and Aliabadi [15] report E = 406.89 GPa and ν = 0.23 considering a microstructure composed by 20 grains and E = 400.9 GPa and ν = 0.24, for 40 grains.

5 Conclusions

In this paper, a multiregion formulation of the Boundary Element Method is applied to polycrystalline silicon carbide and alumina microscales to determine their apparent macroscopic elastic properties. A two-dimensional model is adopted to represent the three-dimensional behavior of the grains within the microstructure, assuming plane strain and varying the material axis coinciding with the geometric z axis. Simulations are performed for

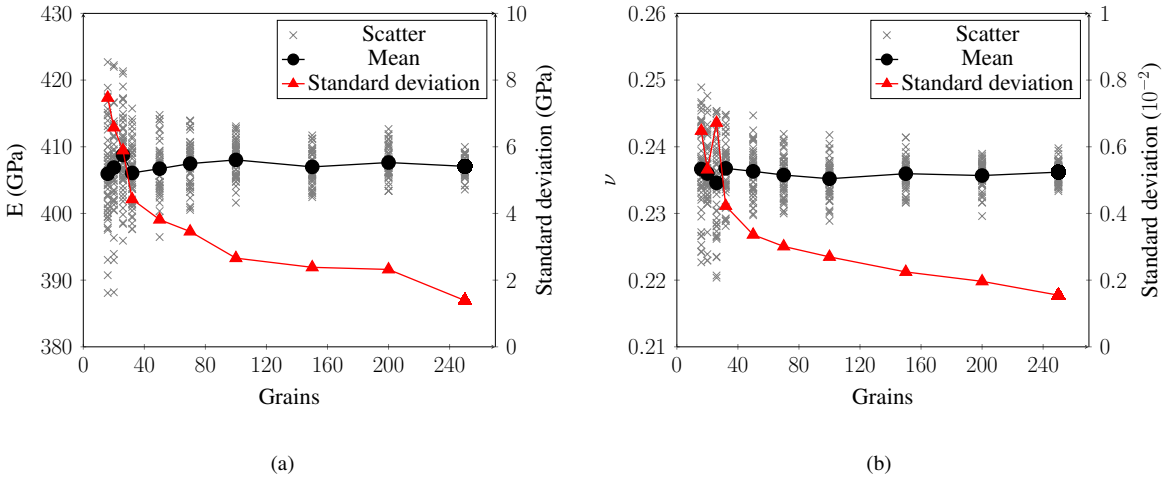


Figure 6. Effective properties of alumina, being (a) elastic modulus and (b) Poisson ratio

different microstructures, considering 16, 20, 26, 32, 50, 70, 100, 150, 200 and 250 grains. Figures 5 and 6 demonstrate that the formulation correctly evaluates the effective properties of SiC and Al_2O_3, in terms of elastic modulus and Poisson ratio, since the results present good agreement with those reported in the literature. When evaluating the different microstructures, it is possible to observe that the average value of the effective properties presented little variation throughout the simulations. For silicon carbide, the average elastic modulus varied by 2 GPa, while Poisson ratio varied by 0.0013. For alumina, the average elastic modulus varied by 4 GPa and Poisson ratio, by 0.0023. In both cases, microstructures composed of 70 grains are capable of representing the mechanical behavior of the polycrystalline aggregate, with standard deviations close to 3.5 GPa for the elastic modulus and 0.003 for Poisson ratio.

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