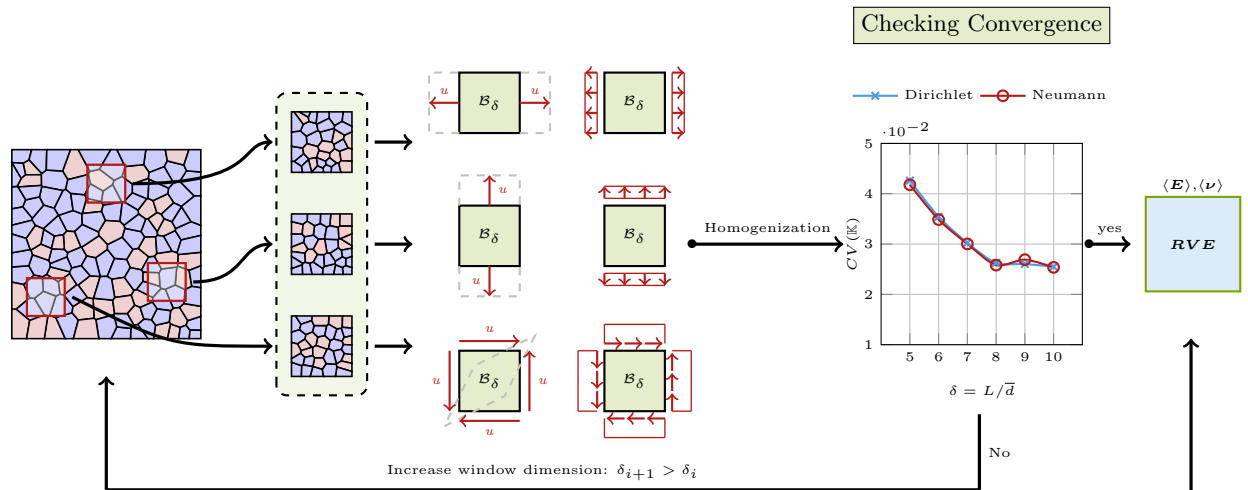


Graphical Abstract

Fast Statistical Homogenization Procedure for estimation of effective properties of Ceramic Matrix Composites (CMC) with random microstructure

Marco Pingaro, Maria Laura De Bellis, Emanuele Reccia, Patrizia Trovalusci, Tomasz Sadowski



Experimental campaign



Highlights

Fast Statistical Homogenization Procedure for estimation of effective properties of Ceramic Matrix Composites (CMC) with random microstructure

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- Homogenization of random Ceramic Matrix Composites (CMC)
- Fast identification of the homogenized moduli with the Virtual Element Method
- Parametric analysis

Fast Statistical Homogenization Procedure for estimation of effective properties of Ceramic Matrix Composites (CMC) with random microstructure

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Abstract

The modern polycrystalline composite materials have a complex internal structure consisting of different phases and interfaces with random distribution. Relevant examples are $\text{Al}_2\text{O}_3/\text{ZrO}_2$, i.e. alumina/zirconia composites, widely used as structural materials with applications ranging from aerospace to bio-engineering. Depending on the phases content and on the grain size a broad range of material characteristics, among which elastic constants, can be obtained.

With the aim of characterizing this class of materials, we exploit a numerical Fast Statistical Homogenization Procedure (FSHP) in order to both estimate the size of the Representative Volume Elements (RVE) and the effective elastic properties, assuming a linear elastic material behaviour.

The 2-D analyses are performed considering a microstructure inspired by images of real portions of the $\text{Al}_2\text{O}_3/\text{ZrO}_2$ composite obtained from a scanning electron microscope. The recent Virtual Element Method is used in combination with the FSHP approach to numerically solve boundary value problems. Different volume contents of phases are considered ranging from pure Alumina to pure zirconia. The results are useful to reliably characterize

such materials in the elastic range taking into account the role played by random distribution of grains.

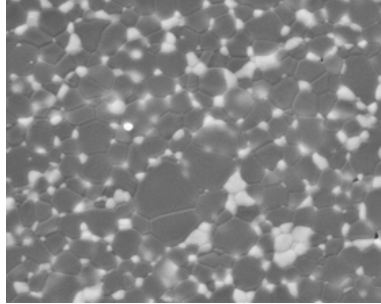
Keywords: Ceramic materials, Random materials, Homogenization, Virtual Element Method

1. Introduction

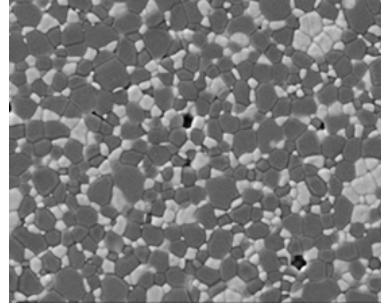
Ceramic matrix composites (CMCs) are a wide class of composites made either by ceramic particles or short/long fibers randomly embedded in a ceramic matrix, or even polycrystalline or also layered composites. They have been designed to overcome the well-known limitations exhibited by standard ceramics used in technical applications, especially related to fragile fracture behaviour both in the presence of mechanical or thermal loads [1]. The addition of ceramic particles or fibers has, indeed, the beneficial effect of increasing the fracture toughness, possibly causing a transition from a fragile to a ductile fracture, and increasing the thermal shock resistance of the composite. On the other hand, the composite material still retains the positive characteristics of the ceramic matrix such as the high strength and Young modulus. Applications include heat shield systems for space vehicles, brake disks, slide bearings, components for high-temperature gas turbines, cutting tools and components for burners, among others [2, 3, 4, 5].

A noteworthy example of a polycrystalline CMC certainly is alumina and phase-stabilized zirconia $\text{Al}_2\text{O}_3/\text{ZrO}_2$ (with different volume contents), see [6]. The considered composite strikes a good balance between positive features of both alumina, i.e. high hardness and low age susceptibility, and zirconia, i.e. high fracture toughness and resistance to subcritical crack growth, see [7, 8]. The $\text{Al}_2\text{O}_3/\text{ZrO}_2$ composite is characterized by a complex internal structure in which grains of either alumina or zirconia of different sizes (ranging from $0.2\mu\text{m}$ to $2\mu\text{m}$) are randomly distributed to form a polycrystal (see Fig.1). Its mechanical characterization has aroused much interest in the scientific community, as demonstrated by [9, 10, 11], with the ultimate aim of designing optimized materials, able to meet high-tech needs.

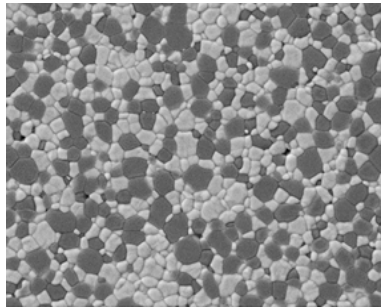
In this paper the focus is on reliably evaluating the effective elastic properties of $\text{Al}_2\text{O}_3/\text{ZrO}_2$, for different volume contents, taking into account the effect of randomness in the micromechanical topology. For this reason we exploit the so-called Fast Statistical Homogenization Procedure in combination with Virtual Element Method, as conceived in [12, 13], to achieve the objective of



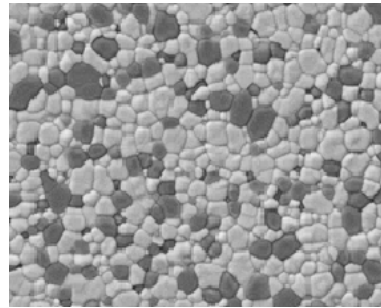
(a) $\text{Al}_2\text{O}_3/\text{ZrO}_2(20\text{-wc})$; distribution of grain sizes - $0.41 \mu\text{m} \pm 0.22$ - Al_2O_3 $0.17 \mu\text{m} \pm 0.06$ - ZrO_2



(b) $\text{Al}_2\text{O}_3/\text{ZrO}_2(20\text{-wc})$; distribution of grain sizes - $0.26 \mu\text{m} \pm 0.11$ - Al_2O_3 $0.22 \mu\text{m} \pm 0.06$ - ZrO_2



(c) $\text{Al}_2\text{O}_3/\text{ZrO}_2(20\text{-wc})$; distribution of grain sizes - $0.24 \mu\text{m} \pm 0.07$ - Al_2O_3 $0.22 \mu\text{m} \pm 0.06$ - ZrO_2



(d) $\text{Al}_2\text{O}_3/\text{ZrO}_2(20\text{-wc})$; distribution of grain sizes - $0.25 \mu\text{m} \pm 0.07$ - Al_2O_3 $0.22 \mu\text{m} \pm 0.06$ - ZrO_2

Figure 1: Microstructure of analysed ceramic material. Light and dark areas represent ZrO_2 and Al_2O_3 , respectively.

32 a comprehensive elastic characterization of the composites, for a wide range
33 of volume fractions, exploiting a numerical tool that has been proven to be
34 easy to use and fast.

35 Within the framework of a first order computational homogenization scheme,
36 both the equivalent elastic moduli and the characteristic size of the Repre-
37 sentative Volume Element are found by developing bounds of the effective
38 response, obtained by solving Boundary Value Problems with either Dirichlet
39 or Neumann boundary conditions [14, 15], as in [16, 17, 18] in the context of
40 micropolar continua.

41 Here the numerical strategy of solution is the very recent Virtual Element
42 Method, [19, 20], which has established itself in recent years as a viable alter-
43 native to Finite Element Method for a wide range of mechanical applications
44 [21, 22, 23, 24, 25, 26]. One of the key advantages is the high flexibility in the
45 number of nodes and shape of elements, so that it seems a very natural tool
46 for materials with polycrystalline microstructures [27] since each grain can
47 be discretized with only one virtual element of generic shape. **There are other**
48 **methods in the literature that can deal with polygonal elements to mimic the**
49 **natural shape of each micro-grain of the material, such as Polygonal Finite**
50 **Elements [28, 29, 30, 31, 32], Voronoi cell Finite Element Method [33, 34, 35]**
51 **and Trefftz-Lekhnitskii Grains (TLGs) [36].**

52 The statistical homogenization procedure is based on: **i) assuming that**
53 **the microstructure satisfies the hypothesis of statistical homogeneity and**
54 **isotropy, combined with the mean-ergodicity; ii) defining realizations of the**
55 random composite, sampled in a Monte-Carlo sense, defined as Statistical
56 Volume Elements of increasing characteristic sizes; **iii) solving properly con-**
57 **ceived boundary problems and evaluating overall mechanical information re-**
58 **lated both to arithmetic mean and dispersion of results; iv) repeating the**
59 procedure up to a convergence criterion is satisfied.

60 Numerical examples are first devoted to a parametric analysis aimed at char-
61 acterizing the $\text{Al}_2\text{O}_3/\text{ZrO}_2$ composite for a set of volume contents ranging
62 from (20%) Al_2O_3 /(80%) ZrO_2 up to (80%) Al_2O_3 /(20%) ZrO_2 . Afterwards
63 a comparison between numerical and experimental results, collected in [8],
64 confirms the reliability of the proposed procedure.

65 The paper is organized as follows. Section 2 presents an overview of the
66 Fast Statistical Homogenization procedure. In Section 3 numerical examples
67 are presented and critically discussed. Finally in Section 4 conclusions are
68 drawn.

69 **2. Fast Statistical Homogenization Procedure (FSHP)**

70 The main aim of this section is to retrace the so-called Fast Statistical
71 Homogenization Procedure (FSHP), already developed by the authors in
72 [12, 13] for particulate composites with circular inclusions, and here modi-
73 fied for taking into account the peculiar structure of the CMC composites
74 characterised by random geometry of the particles besides random positions.
75 The original statistical procedure has been, indeed, conceived for a particular
76 topology, i.e. composites made of circular inclusions, representative of fibers,
77 randomly dispersed in a second phase, called matrix (Fig. 2(a)). Afterword,
78 it has been adapted to model polycrystalline materials bounded by thin inter-
79 faces in which the grains and interfaces zone play the role of inclusions
80 and the matrix, respectively (Fig. 2(b)). Here, focus is on modelling the
81 micro-structure of bi-phase polycrystalline material (Fig. 2(c)).
82 In what follows, the key ideas of the statistical homogenization procedure
83 are briefly summarized and specialized to the materials at hand.

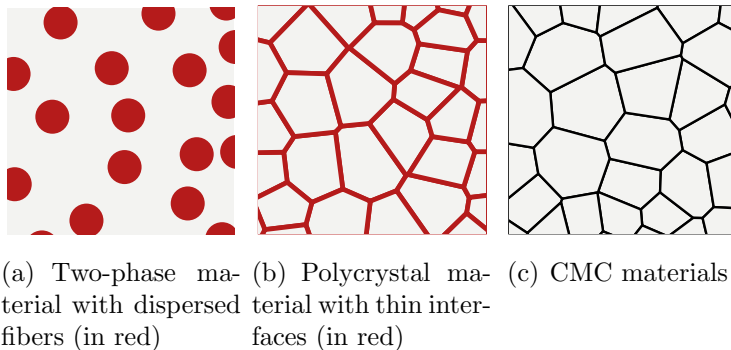


Figure 2: Different models of heterogeneous material taken into account by FSHP.

84

85 *2.1. First order computational homogenization*

A classical energy-based computational homogenization approach [37, 38] is used in combination with the Virtual Element Method to estimate the components of the overall elastic tensor related to realizations of the random CMC Alumina/Zirconia.

In order to perform the homogenization, we describe the material at two

scales of interest: the microscopic and the macroscopic levels. At the microscopic level, the heterogeneous material is represented in detail, accounting for each constituent in terms of geometry and constitutive behaviour. At the macroscopic level the composite material is ideally replaced by an equivalent material whose global behaviour is representative of the actual heterogeneous material. The governing equations are formally the same as those defined at the microscopic level, except for the constitutive law that is not ‘a priori’ defined at the macroscopic level, but directly descends from the lower level as result of the homogenization procedure. In the following, lower case letters are always related to the micro-scale, while upper case letters to the macro-scale.

In the present case of non periodic composite materials and in view of the statistical homogenization procedure, it is useful to introduce a scale parameter $\delta = L/\bar{d}$ defined, at the microscopic scale, as the ratio between the edge of a square test window L , and the characteristic dimension \bar{d} of a grain. We refer to a linearized two-dimensional framework. At the lower level each material phase is characterized by linear elastic isotropic behaviour with the stress–strain relations written as:

$$\boldsymbol{\sigma} = 2\mu \boldsymbol{\varepsilon} + \lambda \operatorname{tr}(\boldsymbol{\varepsilon}) \mathbf{I} \quad (1)$$

where $\boldsymbol{\varepsilon}$ and $\boldsymbol{\sigma}$ are micro-strain and micro-stress tensors, λ and μ are the Lamé constants, and \mathbf{I} is the identity matrix. At the macroscopic level, the general anisotropic stress–strain relations, read:

$$\boldsymbol{\Sigma} = \mathbb{C} \mathbf{E} , \quad (2)$$

where \mathbf{E} , $\boldsymbol{\Sigma}$ are the macro-strain and macro-stress tensors and \mathbb{C} is the homogenized material fourth order tensor that contains the homogenized moduli:

$$\mathbb{C} = \begin{bmatrix} \mathbb{C}_{1111} & \mathbb{C}_{1122} & \mathbb{C}_{1112} \\ \mathbb{C}_{2211} & \mathbb{C}_{2222} & \mathbb{C}_{2212} \\ \mathbb{C}_{1211} & \mathbb{C}_{1222} & \mathbb{C}_{1212} \end{bmatrix} , \quad (3)$$

i.e. the components of the macroscopic elastic tensor obtained via a homogenization procedure based on the Hill macro-homogeneity condition [39]:

$$\boldsymbol{\Sigma} \cdot \mathbf{E} = \frac{1}{A_\delta} \int_{\mathcal{B}_\delta} \boldsymbol{\sigma} \cdot \boldsymbol{\varepsilon} dA, \quad (4)$$

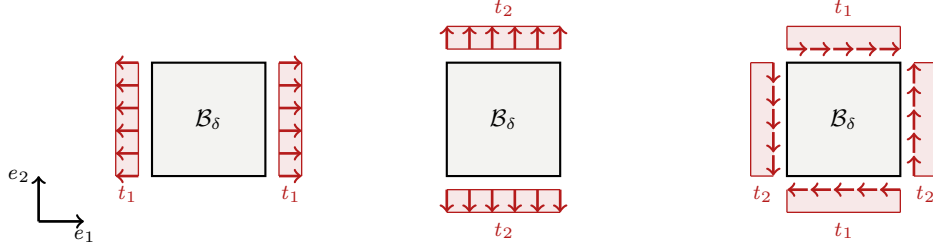


Figure 3: Neumann boundary conditions applied on the window \mathcal{B}_δ

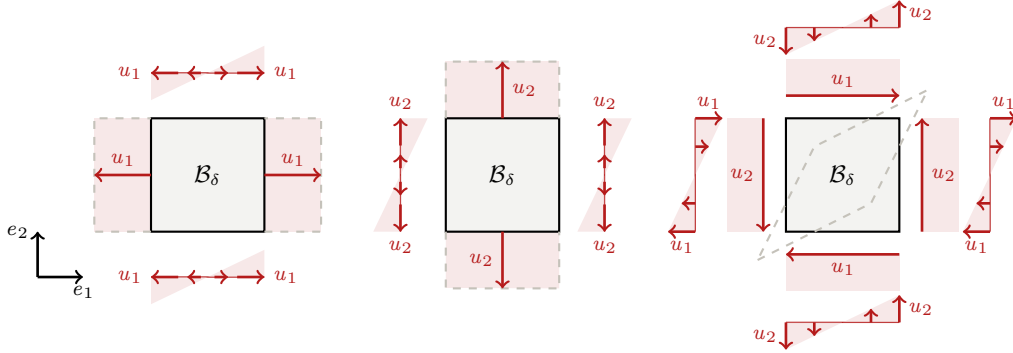


Figure 4: Dirichlet boundary conditions applied on the window \mathcal{B}_δ

86 which states an energy equivalence between the macroscopic point and the
 87 corresponding domain (test window), \mathcal{B}_δ , occupying a region of area A_δ at
 88 the microscopic level.

The homogenization procedure is based on the solution of properly defined boundary value problems at the microscopic level with Dirichlet (Fig. 4) and Neumann (Fig. 3) boundary conditions on the boundary $\partial\mathcal{B}_\delta$, directly deriving from the fulfilment of the macro-homogeneity condition, Eq. (4). We focus on a 2-D problem and assume plane strain conditions. The Dirichlet and Neumann BCs reads, respectively:

$$\begin{aligned} \mathbf{u} &= \mathbf{E} \mathbf{x}, & \text{on } \partial\mathcal{B}_\delta \\ \mathbf{t} &= \boldsymbol{\Sigma} \mathbf{n}, & \text{on } \partial\mathcal{B}_\delta \end{aligned} \quad (5)$$

89 \mathbf{u} being the displacement vector and \mathbf{x} the coordinates of the generic point
 90 on the boundary, $\partial\mathcal{B}_\delta$, with respect to a reference system with origin in the

91 geometric center of the test window \mathcal{B}_δ . \mathbf{t} is the traction vector and \mathbf{n} the
 92 outward normal to $\partial\mathcal{B}_\delta$.

93 As already shown in [27], the geometrical features of a polycrystalline
 94 material are particularly suitable for using the Virtual Element Method as a
 95 numerical tool for solving Boundary Value Problems at the microscopic scale.
 96 In this case, indeed, the microstructure can be satisfactorily modeled with
 97 a randomly generated centroidal Voronoi tessellation (CVT) and it can be
 98 directly used as a computational mesh. As is well known, in fact, the recent
 99 numerical tool of the VEM permits to use single polygonal element for the
 100 grains (Fig. 5b), avoiding internal meshing, with consequent high reduction
 101 of the computational burden with respect to finite elements.

102 Note that at this stage, for the sake of simplicity, the average dimension \bar{d}
 103 of grains is kept constant, but a straightforward modification to account for
 different sizes is possible. The computational strategies adopted are aimed

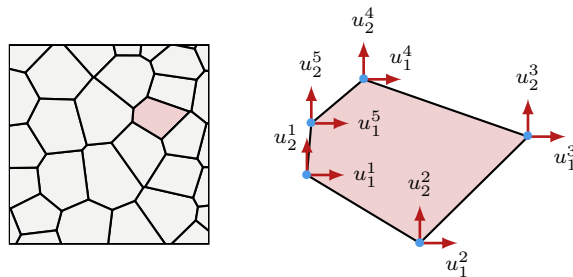


Figure 5: Example of microstructure modelled via CVT (left) obtained by PolyMesher [40] and Virtual Element extract to the mesh (right)

104
 105 at making the statistical homogenization process as efficient as possible for
 106 solving a series (hundreds) of boundary value problems (BVPs), required
 107 by the statistical homogenization procedure and to rapidly converge to the
 108 RVE solution. The capability of the VEM in delivering reliable estimations
 109 of overall elastic moduli, despite the use of very coarse meshes (with conse-
 110 quent important savings in terms of computational burden), has been already
 111 assessed in [27, 12].

112 2.2. Statistical Homogenization

113 FSHP is based on the statistical homogenization procedure proposed in
 114 [41], then developed for micropolar continua in [17] and recently automatized
 115 in [12, 13] and briefly described in Section 1.

116 The proposed homogenization procedure is conceived both for evaluating
117 the homogenized elastic parameters of a non-periodic heterogeneous mate-
118 rial, and for **identifying** the Representative Volume Element (RVE), that in
119 the absence of a repetitive micro-structure is not known a priori.

120 According to the approach presented in [17], as well as in [42, 43], **it**
121 **is assumed the hypothesis of statistical homogeneity and isotropy combined**
122 **with the mean-ergodicity of the microstructure.** In this framework, the pre-
123 sented procedure requires the statistical definition of a number of realizations
124 called Statistical Volume Elements (SVEs), representing the micro-structure,
125 sampled in a Monte Carlo sense, which allows for determining series of scale-
126 dependent upper and lower bounds for the overall elastic moduli and to ap-
127 proach the RVE size, δ_{RVE} , using a statistical stopping criterion, which is
128 based on the variation of the average elastic moduli.

129 All steps of the homogenization procedure are completely integrated in
130 the FSHP and they are described below.

131 Step 1 Input: Set the average dimension of the grains \bar{d} and define the dimen-
132 sionless scale factor $\delta = L/\bar{d}$. Fix the mechanical parameters of each
133 phase: Young modulus and Poisson coefficients of each phase E_i and ν_i
134 , $i=1,2$. Set the minimum number of simulations for convergence, N^{lim} ,
135 and a tolerance parameter, Tol , based on data dispersion, as defined
136 in above.

137 Step 2 Input: initialize the window size, $L = L_0$, and number of simulations,
138 $N = N_0$.

139 Step 3 Realizations: generate a random polygonal mesh with average dimen-
140 sion of grains \bar{d} calling the available **MATLAB**[®] program **PolyMesher** de-
141 veloped by [40]. Each realization is supposed to be independent from
142 any previous one. Based on volume fractions, mechanical parameters
143 are randomly assigned to grains. **In order to avoid abnormal boundary**
144 **layers related to the artifact of generating the Voronoi tessellations from**
145 **realizations of homogeneous random point fields created only within**
146 **the considered test windows, we generate the realizations used in the**
147 **numerical simulations by cutting out smaller windows.** Examples of
148 realization of the micro-structure and the related generated mesh for
149 circular and polycrystal inclusions are shown in Figs. 2(a)-2(b). In Fig.
150 6 a realization obtained by FSHP for different windows size has been
151 plotted, **highlighting in red the cutting windows.**

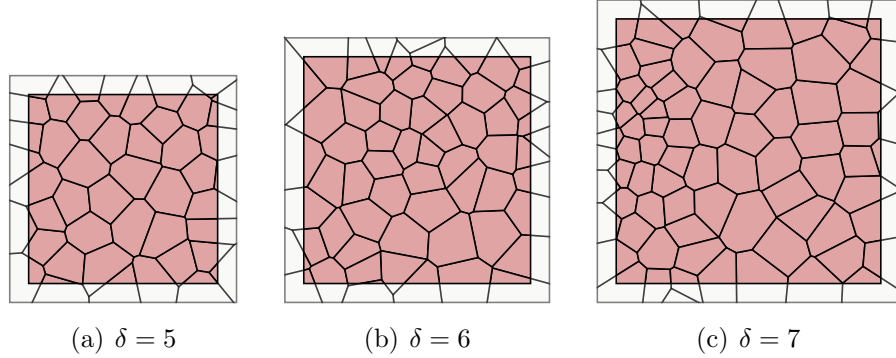


Figure 6: Example of realizations obtained by FSHP for different window size $\delta = L/\bar{d}$ with in red highlighted the cutting windows.

152 Step 4 Generate/Solve: for each SVE, generate the relative mesh and solve
 153 both the Dirichlet and Neumann (Eq. (5)) BVP, and compute the ho-
 154 mogenized constitutive parameters.

Step 5 Compute: the bulk modulus

$$\mathbb{K} = ((\mathbb{C}_{1122} + \mathbb{C}_{2211})/2 + \mathbb{C}_{1212})/6 ,$$

evaluate the average bulk modulus, $\langle \mathbb{K} \rangle_\delta$, the relative standard deviation $\sigma(\langle \mathbb{K} \rangle_\delta)$ and variation coefficient $CV(\langle \mathbb{K} \rangle_\delta)$. Then compute

$$N_i = (1.96 \sigma(\langle \mathbb{K} \rangle_\delta) / (\langle \mathbb{K} \rangle_\delta Tol))^2 , \quad (6)$$

155 which ensures that the confidence interval of the average homogenized
 156 constitutive parameter set at 95%, evaluated over the normal standard
 157 distribution, is within the tolerance allowed, Tol . Repeat Steps 3-4
 158 until $N_i \leq N^{lim}$.

159 Step 6 Checking: if the number of realizations necessary for ensuring the re-
 160 quirement at Step 5 is small enough, stop the procedure. We choose
 161 as the number of realizations necessary the largest unfavourable num-
 162 ber between those obtained by solving BVPs of Neumann or Dirichlet.
 163 Otherwise choose an increased value of δ and go to Step 3.

164 The fulfilment of the requirement at Step 6 means that the values of the
 165 homogenized constitutive coefficients are distributed around their averages

166 with a vanishing variation coefficient, and that the RVE size is achieved. The
167 effective homogenized elastic moduli can be determined as the **arithmetic**
168 **mean** value between the Dirichlet (upper) and Neumann (lower) bounds at
169 the convergence window (RVE).

170 The statistical convergence criterion adopted is based on a 95% confidence
171 level of the Normal Standard distribution, which provides the number N
172 of realizations at which **it** is possible to stop the simulations for a given
173 window size δ . When this number is small enough, the average values of the
174 effective moduli converge and the RVE size is achieved. This circumstance
175 also corresponds to reaching the minimum window size δ_{RVE} for which the
176 estimated homogenized moduli remain constant, within a tolerance interval
177 less than 0.5% for both the Dirichlet and Neumann solutions. The minimum
178 number of simulations, N^{lim} , and the tolerance parameter, Tol , are chosen
179 in order to define a narrow confidence interval for the average and to obtain
180 a reliable convergence criterion. The adopted statistical criterion allows us
181 to detect the RVE size also when the Dirichlet and Neumann solutions do
182 not tend to the same value. The values of the tolerance are assumed as a
183 function of the data dispersion [17].

184 **3. Identification of Alumina/Zirconia properties**

185 This session is devoted to numerical applications aimed both at charac-
186 terizing the elastic properties of the polycrystalline composite at hand for
187 different contents of Alumina/Zirconia and at identifying the dimension of
188 the RVE. In Section 3.1 a parametric analysis is carried out and elastic
189 homogenized moduli are directly compared with classical upper and lower
190 bound estimates. Section 3.2, on the other hand, presents a comparison with
191 experimental results in [8].

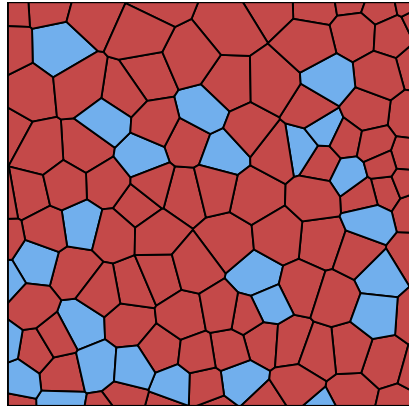
192 *3.1. Comparison with Voigt and Reuss bounds*

193 The Fast Statistical procedure is applied to characterize the elastic re-
194 sponse of the Alumina/Zirconia CMC material in terms of first order ho-
195 mogenized moduli taking into account the influence of randomness in the
196 microstructural topology. Results are compared with the well known up-
197 per (Voigt) and lower (Reuss) bounds estimated using the so-called rule of
198 mixture and inverse rule of mixture, respectively.

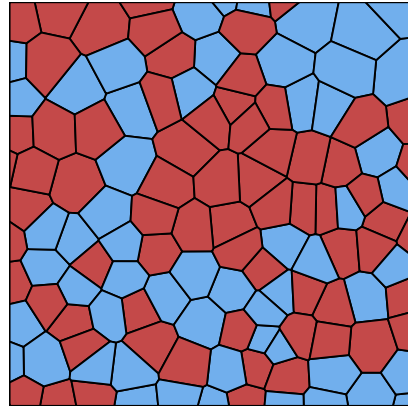
Table 1: Properties of Al_2O_3 and ZrO_2 at room temperature as in [44]

Composite component	E [GPa]	ν [/]
Al_2O_3	400	0.22
ZrO_2	200	0.25

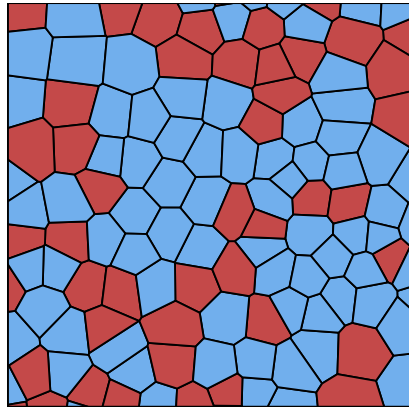
199 Each phase is assumed to behave as a homogeneous linear elastic material.
200 Their properties, borrowed from [44], are reported in Table1. Regarding the
201 dimension of the grains, here we assumed an average dimension $\bar{d} = 5\mu m$.
We consider four different Al_2O_3/ZrO_2 composites characterized by volume fraction $\rho_{Al_2O_3}$ of Alumina in the range 20% to 80%. Figure 7 shows an example of realizations corresponding the four type of materials examined for the window $\delta = 8$. From the homogenization procedure it emerges that the overall behaviour of the composite material does not significantly differ from that of an equivalent isotropic material. In Figure 8(a) and (b) the Dirichlet and the Neumann solutions in terms of homogenized bulk modulus $\langle \mathbb{K} \rangle$ are plotted considering the four values of volume fractions and for different window sizes δ ranging from 5 to 10. As expected, the material tends to become stiffer as the volume content of alumina increases. Dirichlet and Neumann solutions deliver upper and lower bounds, respectively. Applying the convergence criterion in Eq. 6, it emerges that results reach the convergence values at $\delta = 10$, corresponding to the dimension of the RVE. Note that, due to the low material contrast between alumina and zirconia small variations of $\langle \mathbb{K} \rangle$ are observed as δ increases. Moreover, the convergence trend for the different materials depends on the different dispersion of results, as shown in Figs. 9, where the Coefficient of Variation, CV, is plotted versus δ for Dirichlet (blue solid line) and Neumann (red solid line) solutions. As the volume fraction of alumina increases, with the same window size lower values of CV are reached for both Dirichlet and Neumann boundary conditions. The reliability of the proposed procedure is verified by comparing the obtained homogenized moduli with results of well established rule of mixture and inverse rule of mixture, providing upper and lower bounds of homogenized elastic moduli. Considering the homogenized bulk modulus and the composite alumina-zirconia composite characterized by alumina volume fraction $\rho_{Al_2O_3}$, the upper bound



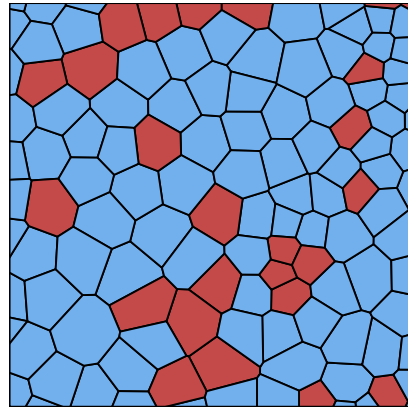
(a) Al_2O_3 20%



(b) Al_2O_3 40%



(c) Al_2O_3 60%



(d) Al_2O_3 80%

Figure 7: Example of realization with different level of Alumina Al_2O_3 and Zirconia ZrO_2 for window dimension $\delta = L/\bar{d} = 9$: Alumina and Zirconia grains are depicted in blue and red color, respectively

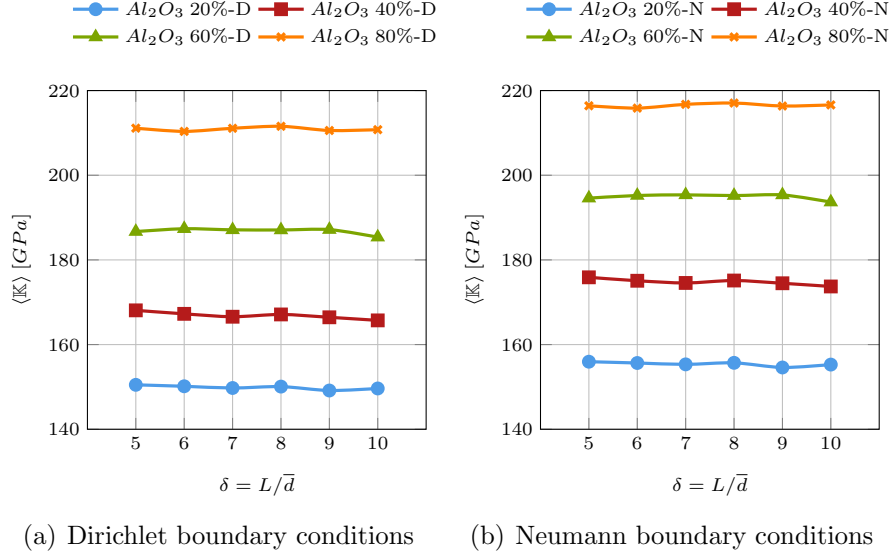


Figure 8: Homogenized Bulk modulus $\langle \mathbb{K} \rangle$ with varying the window dimension $\delta = L/\bar{d}$

solution, obtained using the Voigt model, results as

$$\langle \mathbb{K} \rangle_{Al_2O_3/ZrO_2}^{upper} = \langle \mathbb{K} \rangle_{Al_2O_3} \rho_{Al_2O_3} + \langle \mathbb{K} \rangle_{ZrO_2} (1 - \rho_{Al_2O_3}) \quad (7)$$

as well as the lower bound solution, obtained via the Reuss model, reads as

$$\langle \mathbb{K} \rangle_{Al_2O_3/ZrO_2}^{lower} = \left(\frac{\rho_{Al_2O_3}}{\langle \mathbb{K} \rangle_{Al_2O_3}} + \frac{1 - \rho_{Al_2O_3}}{\langle \mathbb{K} \rangle_{ZrO_2}} \right)^{-1} \quad (8)$$

202 In Figure 10 the values of homogenized bulk modulus corresponding to RVEs
 203 are plotted as the volume content of alumina varies. The extremal cases cor-
 204 respond to pure zirconia and pure alumina. Blue and red curves are referred
 205 to Dirichlet and Neumann solutions obtained with the Fast Statistical Ho-
 206 mogenization procedure, while dashed black and orange curves are referred
 207 to upper and lower bounds resulting from rule of mixture and inverse rule of
 208 mixture, respectively. As expected, it is observed that the results obtained
 209 from the proposed homogenization procedure fall within the bounds.

210 Furthermore, the same investigation has been carried out considering the
 211 homogenized Poisson's ratio corresponding to the RVE. As emerges from Fig-
 212 ure 11, where the four curves have the same meaning as in Figure 10, slight

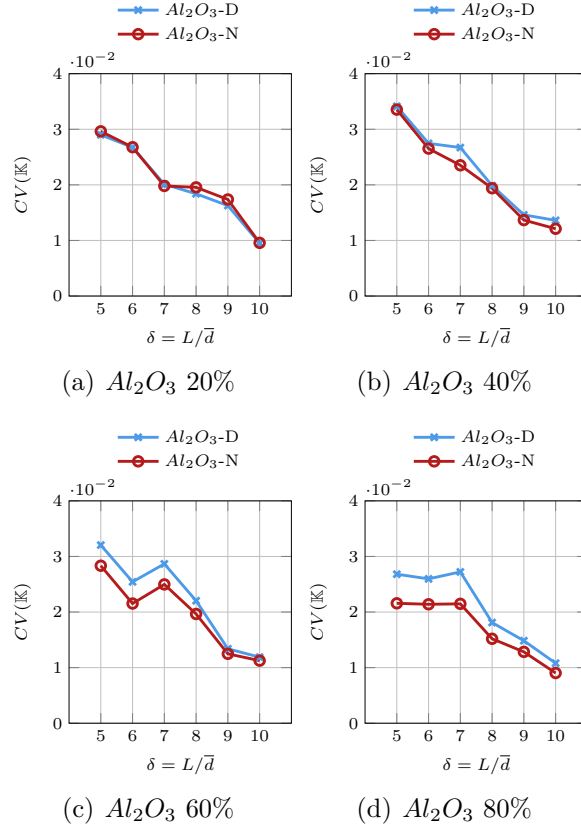


Figure 9: Coefficient of variation $CV(\mathbb{K})$ for different contents of Al_2O_3 : Dirichlet boundary condition in blue line and Neumann boundary conditions in red line

213 deviations from the upper and lower bounds are observed pointing out that
 214 the proposed statistical procedure confirms to provide reliable results.

215 3.2. Comparison with experimental results

216 As a second investigation, the numerical procedure is validated against
 217 experimental results of [8] corresponding to four different alumina/zirconia
 218 composites. In the referred paper a comprehensive experimental campaign
 219 has been carried out with the aim of determining a wide set of material
 220 properties as fracture toughness, bending strength, Young's modulus, hard-
 221 ness and subcritical crack growth. Examples of tests performed in the Lublin
 222 laboratories are shown in Fig.12. In this context, we are interested in homog-
 223 enized Young modulus. In line with [8], we consider for the alumina, Al_2O_3 ,

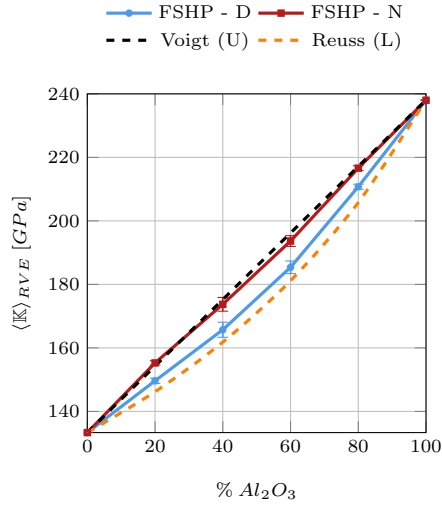


Figure 10: Homogenized Bulk modulus $\langle \mathbb{K} \rangle_{RVE}$ at convergence for different level of percentage ρ of Al_2O_3

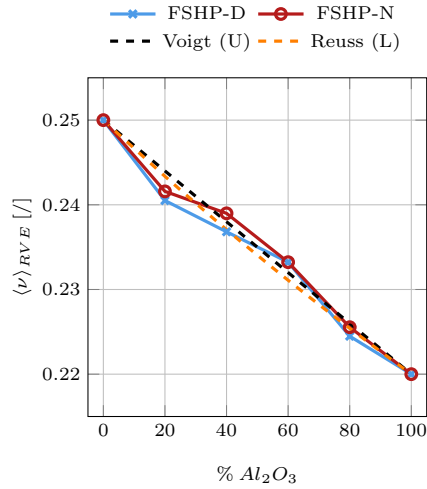
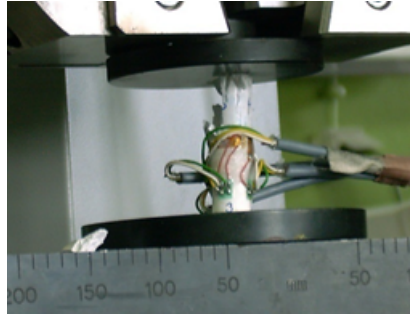


Figure 11: Homogenized Poisson coefficient $\langle \nu \rangle_{RVE}$ at convergence for different level of percentage ρ of Al_2O_3

224 Young modulus $E = 370$ GPa and Poisson's ratio $\nu = 0.22$, while for zirconia,
 225 ZrO_2 , Young modulus $E = 205$ GPa and Poisson's ratio $\nu = 0.25$. In Fig-



(a) Compression test



(b) Example of the specimen (c) Three bending point test of the specimen

Figure 12: Example of tests campaign performed at Lublin laboratories [8].

226 ure 13 the homogenized Young moduli as the volume content of Al_2O_3 varies
 227 are plotted considering both experimental results and those obtained via the
 228 numerical statistical procedure at hand. A very good agreement is found,
 229 confirming that the FSHP is able to accurately reproduce experimental re-
 230 sults.

231 Finally, in Table 2 the homogenized average components C_{ijkl} of the elastic
 232 fourth order tensor, corresponding to the RVE, are listed for the four values
 233 of Al_2O_3 content. As already mentioned, the overall elastic behaviour can be
 234 described with a good approximation by an isotropic linear elastic equivalent
 235 continuum.

236 4. Final remarks

237 The polycrystalline Al_2O_3/ZrO_2 composite [8] has been characterized in
 238 the linear elastic regime by generalizing a statistical homogenization proce-
 239 dure previously developed by some of the authors [12, 13]. Emphasis is placed
 240 on the influence that randomness in the phase distribution can have on the
 241 equivalent elastic response of the polycrystalline material. The procedure

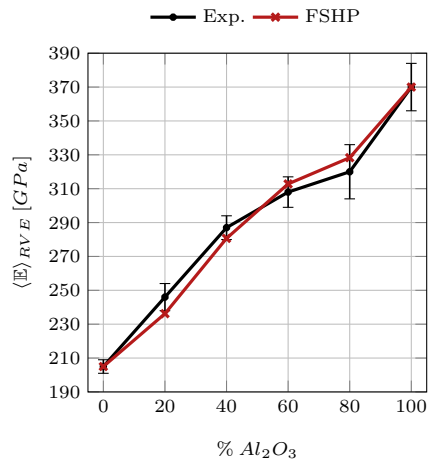


Figure 13: Homogenized Young modulus $\langle E \rangle_{RVE}$ at convergence for different level of percentage ρ of Al_2O_3 (red line) versus experimental test (black line)

242 has the twofold purpose of estimating the elastic moduli via upper and lower
 243 bounds obtained with Dirichlet and Neumann type boundary conditions and
 244 identifying the dimension of the RVE corresponding to the composite mate-
 245 rial. The numerical tool exploited to solve boundary value problems is the
 246 recent Virtual Element Method.

247 Numerical investigations are carried out accounting for different phase con-
 248 tents in the composite ranging from pure Alumina to pure Zirconia. A first
 249 investigation highlights that as expected the Neumann and Dirichlet bounds
 250 obtained with the proposed solution fall within upper and lower bounds ob-

Table 2: Homogenized elastic parameters of Al_2O_3/ZrO_2 composite for different level of alumina Al_2O_3 percentage

% Al_2O_3 []	C_{1111} [GPa]	C_{1122} [GPa]	C_{2211} [GPa]	C_{2222} [GPa]	C_{1212} [GPa]
20	279.1555	89.2250	89.2090	279.0855	192.8280
40	306.4810	95.0085	94.9825	307.1135	215.4210
60	362.2085	106.5220	106.5265	361.3640	257.8255
80	377.9210	109.9360	109.9520	377.1985	269.9895

251 tained with Voigt and Reuss models. Given the low contrast between the
252 elastic modules of two phases, the procedure guarantees convergence for rel-
253 atively small testing windows, corresponding to RVEs of rather small dimen-
254 sions, i.e. with a characteristic size equal to approximately 10 times the
255 average grain size. Moreover, it is noted that the homogenized material ex-
256 hibits an overall elastic response that does not significantly differ from the
257 isotropic behaviour.

258 The numerical procedure has been, then, successfully applied to reproduce
259 experimental results related to characterization of Young modulus for a set
260 of Alumina/Zirconia materials which differ in Alumina content.

261 Further developments envisage the investigation of homogenized non-linear
262 constitutive behaviors, possibly accounting for crack onset and development.

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