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A boundary element method for thermo-elastic homogenization of polycrystals

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Abstract. A computational framework for thermo-elastic homogenization of polycrystalline materials is proposed. The formulation is developed at the crystal level and it is based on the explicit Voronoi representation of the micro-morphology. The crystal thermo-elastic equations are formulated in an integral form and numerically treated through the boundary element method. The presence of volume integrals, induced by the inherent physics of the thermo-elastic coupling, is addressed through a Dual Reciprocity Method (DRM), which allows recasting the formulation in terms of boundary integrals only. The developed methodology is applied for estimating the homogenized thermo-elastic constants of two widely employed ceramic materials. The method may find applications in multiscale analysis of polycrystalline structural component.

Introduction

Multiscale materials modelling, which focuses on understanding how mechanisms at different length/time scales interact and contribute to the emerging of materials properties at larger scales, is assuming increasing importance in engineering, thanks to developments in experimental materials nano/micro-characterization, which provide a wealth of detailed information about the materials constituents, and to the larger availability of high performance computing, which provides the means to process all the available information in complex modelling frameworks. This favours the understanding of existing materials and boosts the design of new ones, with desired properties at a given scale, consolidating the *materials-by-design* paradigm [1].

An essential item of multiscale modelling is materials homogenization, which generally focuses on inferring the materials aggregate properties at a given scale from the knowledge of the morphological and constitutive features of material constituents at lower scales. Examples are provided by the techniques focused on predicting the properties of composite materials at the laminate level from the characterization of the individual plies or even, at a lower scale, from the properties of fibers and matrices and their mutual arrangement. An important concept in materials homogenization is that of *representative volume element* that may be defined as a material sample small enough to be considered as a material point at the component scale, but large enough to contain a number of elementary micro-constituents sufficient to characterize the aggregate properties in an average sense, so that no meaningful fluctuations in average materials properties are induced by small variations of the specimen size [2].

In this work, an original framework for computational homogenization of polycrystalline materials, is discussed. Polycrystalline materials, which include metals, alloys, or ceramics, are widely employed in engineering and their properties at the component level emerge from the properties of individual crystals and their interactions. The framework is based on the employment of a multi-region boundary integral formulation for representing the thermo-mechanics of the

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aggregate. Differently from finite element approaches, it allows examining the thermo-elastic problem considering as primary variables only crystal boundary displacements, temperature, tractions and thermal fluxes, promoting remarkable savings in terms of overall number of degrees of freedom and computational storage memory and resolution time, which is of paramount importance for effective multiscale analysis.

This work summarizes the main aspects of the developed framework and reports some homogenization results. The interested readers may access Refs.[3-13] for further details.

Formulation overview

The developed framework is based on: *i*) algorithms for the generation of sets of Voronoi polycrystalline specimens [3,6]; *ii*) robust meshing algorithms able to deal with the statistical features of polycrystalline aggregates [6]; *iii*) a boundary integral representation of the thermo-elastic problem obtained through the *dual reciprocity method* (DRM) [13]; *iv*) algorithms for the discretization and robust numerical integration of the thermo-mechanical boundary integral equations [13]; *iv*) algorithms for the computation of volume averages of the micro-fields, needed for retrieving the *apparent* materials properties and estimating the *effective* ones [13].

Morphology generation/meshing. Voronoi-Laguerre tessellations are employed to represent polycrystalline morphologies retaining the main statistical features of real materials. Open-source packages, e.g. VORO++ (https://math.lbl.gov/voro++/) or NEPER (https://neper.info), are available to generate general 3D tessellations. Specialized algorithms for robust boundary elements meshing are presented in Ref.[6]. *Non-prismatic periodic realizations* are employed in this work, as they remove boundary walls distortions and enhance homogenization convergence.

Boundary integral formulation. Differently from finite elements, the starting point for the formulation is the single-crystal thermo-elastic boundary integral representation

$$c_{ij}(\boldsymbol{x})\, U_j(\boldsymbol{x}) + \int_\Gamma \hat{T}^*_{ij}(\boldsymbol{x},\boldsymbol{y}) U_j(\boldsymbol{y}) d\Gamma = \int_\Gamma \mathrm{U}^*_{ij}(\boldsymbol{x},\boldsymbol{y}) T_j(\boldsymbol{y}) d\Gamma + \int_\Omega \mathrm{U}^*_{ij}(\boldsymbol{x},\boldsymbol{y}) F_j(\boldsymbol{y}) d\Gamma \qquad (1)$$

where: $\boldsymbol{i},\boldsymbol{j}$ =1,…,4; $\boldsymbol{\Gamma}$ and $\boldsymbol{\Omega}$ denote the crystal boundary and domain; *x* and *y* are respectively the *collocation* and *integration* point; $\boldsymbol{U_j}$ and $\boldsymbol{T_j}$ are components of generalized thermo-elastic displacements and tractions respectively, which collect, respectively, components of displacements and the temperature jump and components of mechanical tractions and the thermal flux; $\mathbf{U}^*_{\boldsymbol{ij}}$ and $\widehat{\boldsymbol{T}}^*_{\boldsymbol{ij}}$ are contain combinations of components of the elastic and thermal fundamental solutions, such as to introduce the thermo-elastic coupling in the integral representation, together with the volume terms $\boldsymbol{F_j}$, which contains components of the thermal gradient. In Eq.(1) the first integral on the left-hand side must be intended as Cauchy principal value.

The presence of the volume integral in Eq.(1) requires special consideration: its presence would call for volume discretization, thus reducing the attractiveness of the integral formulation. To retrieve the benefits of a pure *boundary* representation, this integral can be transformed into a sum of boundary integrals employing the dual reciprocity technique described in Ref.[13] and references therein. Once this transformation is performed, the pure boundary integral equations can be employed for modelling the thermo-mechanics of the aggregate: for each grain, they are collocated at the nodes of the boundary mesh and are numerically integrated using the boundary element method. After such operations, discrete systems expressed in terms of generalized thermo-elastic boundary nodal displacements and tractions are associated with each grain; such equations are then coupled with suitable interface continuity/equilibrium equations and with consistent boundary conditions enforced on the overall aggregate producing a system of the form

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$$\begin{bmatrix} \mathbf{A} \\ I \end{bmatrix} \mathbf{X} = \begin{bmatrix} \mathbf{BY} \\ \mathbf{0} \end{bmatrix} \tag{2}$$

where the blocks A and B contain coefficients stemming from the boundary element integration, X and Y collect, respectively, unknown and known nodal components of displacements, temperature, tractions and thermal flux, and I implements the intergranular continuity equations. Eq.(2) is to be solved with sparse-matrix specialized solvers, due to its numerical structure.

Once the numerical solution of the system in Eq.(2) is available, the micro-fields can be solved. The homogenization is performed enforcing periodic thermo-elastic boundary conditions and computing volume averages of stresses and thermal fluxes, which allows retrieving the apparent elastic, conductivity, and thermo-elastic apparent constants. In this work a *statistical computational homogenization* is implemented, which employs both ensemble and volume averages for estimating apparent and effective properties. Assuming ergodicity, ensemble averages of volume averages computed over sets of polycrystals containing a selected number of gains are computed to associate apparent properties with that number of grains; the operation is repeated at increasing number of grains until convergence of the apparent properties is recorded, thus providing an estimate of the material effective properties, see Ref.[13].

Some numerical results

Statistical computational homogenization results about polycrystalline silicon carbide and alumina are presented here. Single crystal properties at room temperature are taken as in Ref.[13] and Fig.(1) shows the convergence of the apparent thermo-elastic constants at increasing number of grains. Ensemble averages are computed over sets of ten realizations and up to 100 grains per realization are considered. The estimated properties always fall within Reuss and Voigt bounds.

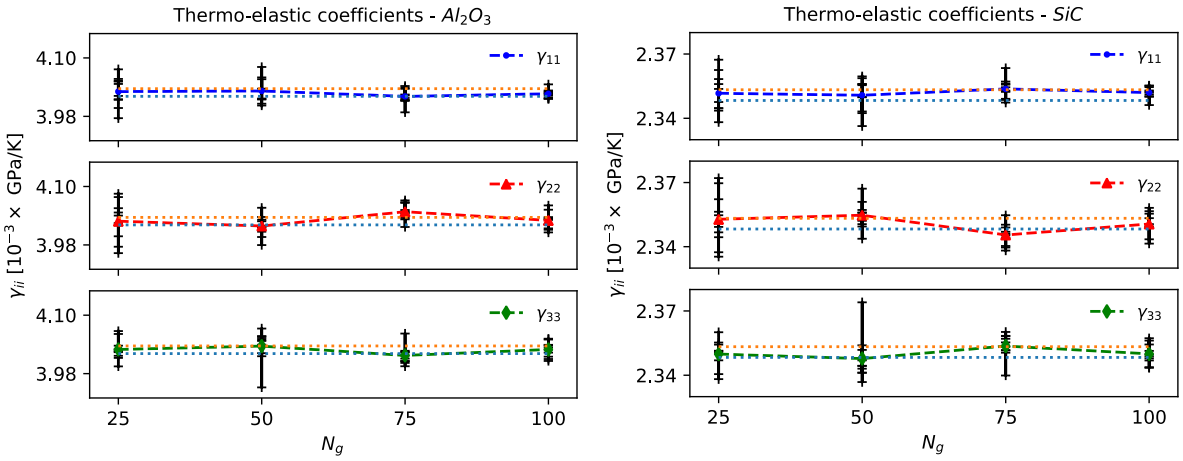

Fig.1: Computational homogenisation results for selected components of thermo-elastic coefficients for polycrystalline alumina and silicon carbide. The + markers identify volume averages over single realisations, the dashed curves correspond to ensemble averages, while the shaded area lies between the Reuss' and Voigt's bounds.

Summary

The development of an original multi-region dual reciprocity boundary elements framework for thermo-elastic homogenization of polycrystalline materials has been discussed, highlighting the benefits offered with respect to other popular approaches. The presented results highlight the effectiveness in estimating materials effective properties. The proposed tool may be employed as component of multiscale analysis tools.

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