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A Model for Polycrystalline Thermo-Mechanical Homogenisation and Micro-Cracking

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Abstract

A grain scale framework for thermo-elastic and micro-cracking analysis of polycrystalline materials is proposed. The polycrystalline morphology is represented through Voronoi tessellations, which retain the main statistical features of polycrystalline materials. The coupled thermo-mechanical response of the grains is modelled using an integral representation for anisotropic thermo-elasticity, which is the numerically addressed through a *dual reciprocity boundary element method*. The continuity of the aggregate is enforced through suitable intergranular thermo-elastic cohesive interfaces that represent the thermo-mechanical degradation through an irreversible damage parameter, which affects both the interface strength and thermal conductivity. Thanks to the features of the underlying formulation, the micro-mechanical thermo-elastic problem is expressed in terms of grain boundary variables only, which simplifies the meshing procedures and reduces the overall number of degrees of freedom and then the numerical cost of the analysis. Preliminary results about thermo-elastic homogenisation are discussed, while the results of micro-cracking simulations will be presented in a forthcoming study.

Keywords: Polycrystalline materials; Thermo-mechanical coupling; Computational micro-mechanics; Multiscale Materials Modelling; Dual Reciprocity Boundary Element Method.

1. Introduction

Modelling of materials at different length and time scales is attracting increasing interest in engineering and science, as it helps understand complex materials mechanisms and enhance the design of tougher and safer materials and structures, Tadmor and Miller (2011). In this context, the present work discusses the development of a computational tool for thermo-elastic homogenisation of polycrystalline materials and for the analysis of polycrystalline micro-cracking induced by thermo-mechanical loading.

Polycrystalline microstructures, at scales ranging from nano- to micro-meters, are exhibited by several classes of materials, including metals, alloys and ceramics, which are widely employed in engineering applications. The mechanical and thermal properties of such materials at the component level emerge from the properties and interactions of the individual crystals, which generally present general anisotropy and orientation in space. A fundamental role in the crystal aggregate behaviour is played by intergranular interfaces, which generally have complex physical-chemical structure and may be the seat of complex phenomena, including damage initiation.

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In the literature, several contributions have addressed grain-scale mechanical modelling of polycrystalline materials, Benedetti and Barbe (2013). One of the most popular approaches for the analysis of polycrystalline aggregates is the finite element method (FEM), often employed in conjunction with crystal plasticity – Roters et al. (2010); Barbe et al. (2001) – and cohesive zone modelling – Espinosa and Zavattieri (2003) – for the representation of complex non-linear material phenomena. Other recent approaches include generalisations of FEM, such as the *virtual element method* (VEM) – Marino et al. (2019); Lo Cascio et al. (2020) – or *phase field* approaches, Emdadi and Asle Zaeem (2021).

The computational tool discussed here is based on the employment of an alternative integral formulation for the representation of the thermo-mechanical polycrystalline problem and of the *boundary element method* (BEM) for its numerical resolution. BEM has been successfully employed in the analysis of polycrystalline problems, both in 2D – Geraci and Aliabadi (2017) – as well as in 3D – Benedetti and Aliabadi (2013a,b, 2015); Benedetti et al. (2016); Gulizzi et al. (2018); Benedetti et al. (2018); Benedetti and Gulizzi (2018); Benedetti et al. (2019); Parrinello et al. (2021). The polycrystalline thermo-mechanical problem has been addressed employing BEM by Geraci and Aliabadi (2018, 2019) in 2D, while Benedetti (2023) developed a formulation for 3D thermo-elastic homogenisation. The attractiveness of such BEM formulations derives from *i*) the pre-processing simplification, *ii*) the reduction in the number of DoFs required with respect to other methods and *iii*) from the employment, as primary variables, of grain-boundary displacements and *tractions*, which favour a natural coupling with cohesive zone modelling. However, in the thermo-elastic case, the coupling between the thermal and elastic field introduces, in the adopted integral formulation, some volume integrals whose presence, if not suitably addressed, cancels the benefits (*i*) and (*ii*) listed above. Such inconvenience may be overcome resorting to the *dual reciprocity method* (DRM) – P. W. Partridge (1991), which allows retrieving a pure boundary formulation, with the associated benefits.

In this work, the extension of the model presented by Benedetti (2023) to polycrystalline micro-cracking analysis, through the adoption of suitable thermo-mechanical cohesive laws is discussed. Some preliminary results about thermo-elastic homogenisation are discussed, while numerical results about micro-cracking analysis will be presented in a forthcoming contribution.

2. Formulation

The proposed formulation is based on different items, namely: *i*) Voronoi-Laguerre tessellation algorithms for representing the polycrystalline morphologies; *ii*) suitable boundary elements discretisation algorithms of such morphologies; *iii*) a *dual reciprocity* boundary integral representation of the thermo-mechanical problem for the individual grains; *iv*) a set of subroutines for the boundary element discretisation and integration of the above boundary integral representation; *v*) a suitable thermo-mechanical cohesive zone model of the intergranular interfaces, to intergranular capture damage initiation and evolution; *vi*) a robust solver for both the linear thermo-elastic problem and the non-linear incremental-iterative thermo-mechanical micro-cracking polycrystalline problem; *vii*) suitable averaging theorems and routines for thermo-elastic homogenisation.

2.1. Generation and discretisation of polycrystalline microstructures

Suitable tessellations able to represent the main statistical features of real polycrystalline materials can be generated using Laguerre-Voronoi algorithms, for which effective and general open-source software packages, such as `VORO++` – Rycroft (2009) – and `NEPER` – Quey et al. (2011) – are available. Once a tessellation is available, a quality boundary element must be generated; in this work triangular/quadrangular semi-discontinuous are generated using the algorithm developed by Gulizzi et al. (2015). Fig.(1) shows an example tessellation and the boundary mesh associated to individual grains.

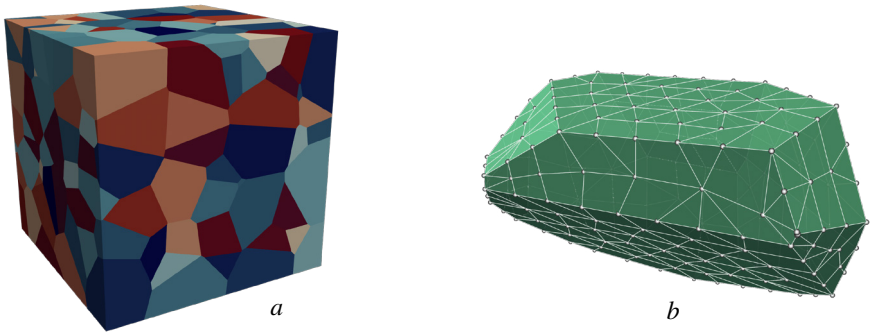

Fig. 1: (a) Example of Voronoi tessellation containing 300 grains; (b) Example of boundary element mesh of a single crystal.

2.2. *Dual Reciprocity Boundary Element Method for the thermo-mechanical analysis of grains*

Once the tessellation and associated mesh are available, thermo-mechanical analysis of individual crystals is built starting from a suitable set of integral equations. In this work, steady state thermo-elastic problems are considered, for which an integral representation is provided as

$$c_{ij}(\boldsymbol{x})\,U_j(\boldsymbol{x}) + \oint_{\Gamma^g} \hat{T}^*_{ij}(\boldsymbol{x},\boldsymbol{y})\,U_j(\boldsymbol{y})d\Gamma_y = \int_{\Gamma^g} U^*_{ij}(\boldsymbol{x},\boldsymbol{y})\,T_j(\boldsymbol{y})d\Gamma_y + \int_{\Omega^g} U^*_{ij}(\boldsymbol{x},\boldsymbol{y})\,F_j(\boldsymbol{y})d\Omega_y \qquad i,j=1,...,4, \quad (1)$$

where: Γ^g and Ω^g represent the boundary and volume of the generic grain g; $\boldsymbol{x}$ and $\boldsymbol{y}$ are the *collocation* and *integration* points, respectively; $\left\{U_j\right\} = \{u_1, u_2, u_3, \theta\}$ is a generalised vector containing the displacement components u_i and the temperature jump θ with respect to a reference temperature T_0; $\left\{T_j\right\} = \{t_1, t_2, t_3, q_n\}$ is a generalised vector containing the components of boundary tractions and thermal flux; $\left\{F_j\right\} = \{-\gamma_{1k}\theta_{,k}, -\gamma_{2k}\theta_{,k}, -\gamma_{3k}\theta_{,k}, 0\}$ is a generalised volume load term depending, if other volume terms such as weight or centrifugal forces may be neglected, only on the temperature gradients; U^*_{ij} and $\hat{T}^*_{ij}$ contain suitable combinations of components of the static elastic and thermal fundamental solutions. In Eq.(1) the thermo-elastic coupling is introduced by the volume terms F_j and by the components of $\hat{T}^*_{ij}$; the symbol $\oint$ represent the Cauchy principal value; and the terms c_{ij} stem from the boundary collocation limiting procedure, see e.g. Aliabadi (2002).

The volume integral in Eq.(1) can be transformed into boundary integrals employing a dual reciprocity representation, i.e.

$$\int_{\Omega^g} U^*_{ij}F_j d\Omega_y + \int_{\Gamma^g} U^*_{ij}\tilde{T}_j d\Gamma_y = \oint_{\Gamma^g} T^*_{ij}\tilde{U}_j d\Gamma_y + c_{ij}\tilde{U}_j(\boldsymbol{x}) \qquad i,j=1,...,4, \quad (2)$$

where $\tilde{U}_j$ and $\tilde{T}_j$ are generalised thermo-elastic displacements and tractions associated to *particular solutions* of the uncoupled thermo-elastic problem $\mathcal{L}^{te}\left(\tilde{\boldsymbol{U}}\right) + \boldsymbol{F} = \boldsymbol{0}$. Since particular solutions are not easily computable, their approximated solutions are built employing radial basis functions, which is typical of dual reciprocity method. Further details can be found in Kögl and Gaul (2003).

Once a DRBEM representation is built, the boundary integral equations can be numerically integrated approximating the generalised displacements and tractions over the boundary elements through shape functions and nodal values and then employing classical quadrature algorithms, taking care in addressing singularities arising when the integration and collocation points coincide. The integration lead, for the generic grains g to discrete equations of the form

$$\mathbf{H}^g_{te}\check{\mathbf{U}}^g = \mathbf{G}^g\check{\mathbf{T}}^g, \quad (3)$$

where $\check{\mathbf{U}}^g$ and $\check{\mathbf{T}}^g$ collect nodal values of generalised displacements and tractions, and the matrices $\mathbf{H}^g_{te}$, and $\mathbf{G}^g$ collect coefficients stemming from the numerical integration. Eq.(3) can be associated to each grain; to restore the integrity of the aggregate, suitable intergranular conditions must be complemented.

2.3. Intergranular evolution: from thermo-mechanical continuity to micro-cracking

The behaviour of the intergranular interfaces is modelled, in the present framework, employing conformal meshes at the contiguous faces of two generic grains a and b, and employing different sets of equations depending on the evolution status of the considered interface region. In general, an intergranular region can be pristine, damage or failed. The interface remains *pristine* as long as the tractions remain below a certain threshold during the loading history; in this case, the generalised tractions equilibrium dictates $T_i^a = T_j^b$, which always hold, also when damage/failure are reached, while the displacements continuity requires $\delta U_i = 0$. When a certain *effective* traction threshold is overcome, the displacement continuity equations are replaced by suitable thermo-mechanical traction-separation laws that, following Özdemir et al. (2010), may be written as

$$T_i = K_{ij}(\omega)\,\delta U_j \qquad i,j = 1,\dots,4 \tag{4}$$

where $\omega \in [0,1]$ represents an irreversible damage parameter that allows tracking the evolution from pristine to failed status. Eq.(4) allows modelling different kinds of interfacial behaviour, either thermo-mechanically coupled or uncoupled. Further details about mechanical and thermo-mechanical cohesive laws can be found in Benedetti and Aliabadi (2013a) and Özdemir et al. (2010) and references therein. An interface region fails when $\omega \to 1$. When this condition is reached, the laws of contact mechanics come into play and the interface can be either in contact stick/slip or separation, with consistent thermo-mechanical jump displacement equations enforced.

2.4. Thermo-mechanical polycrystalline system and its numerical solution

Once the discrete equations for each crystal are written, the boundary conditions on the external walls of the aggregate *and* the interface equations are enforced, the polycrystalline system reads

$$\begin{bmatrix} \mathbf{A}\cdot\mathbf{X} \\ \mathbf{I}_{\mathrm{IG}}(\mathbf{X},\omega) \end{bmatrix} = \begin{bmatrix} \mathbf{B}\cdot\mathbf{Y}(\lambda) \\ \mathbf{0} \end{bmatrix} \qquad \text{with} \qquad \mathbf{A} = \begin{bmatrix} \mathbf{A}^1 & \cdots & \mathbf{0} \\ \vdots & \ddots & \vdots \\ \mathbf{0} & \cdots & \mathbf{A}^{N_g} \end{bmatrix} \qquad \mathbf{B} == \begin{bmatrix} \mathbf{B}^1 & \cdots & \mathbf{0} \\ \vdots & \ddots & \vdots \\ \mathbf{0} & \cdots & \mathbf{B}^{N_g} \end{bmatrix} \tag{5}$$

where the blocks $\mathbf{A}^g$ and $\mathbf{B}^g$, associated with individual crystals, are obtained from Eqs.(3) upon application of the external boundary conditions and the block $\mathbf{I}_{\mathrm{IG}}(\mathbf{X},\omega)$ implements the evolving interface conditions. The system in Eq.(5) is solved through a Newton-Raphson incremental-iterative solver, as discussed for example by Gulizzi et al. (2015). The linear solution steps should be addressed employing specialised linear sparse solvers, being the coefficient matrices highly sparse.

2.5. Thermo-elastic homogenisation

Thermo-elastic steady-state homogenisation can be conducted enforcing suitable generalised macro-strains or temperature variations and then averaging the ensuing elastic stress and and thermal flux components. In this work, statistical homogenisation is performed, so that both *volume* and *ensemble* averages are computed. The reference equations for computing the apparent properties associate with a given morphology are

$$\begin{bmatrix} \langle\boldsymbol{\sigma}\rangle \\ \langle\boldsymbol{q}\rangle \end{bmatrix} = \begin{bmatrix} \boldsymbol{C}^A & \mathbf{0} & \boldsymbol{\gamma}^A \\ \mathbf{0} & \boldsymbol{\kappa}^A & \mathbf{0} \end{bmatrix} \begin{bmatrix} +\langle\boldsymbol{\varepsilon}\rangle \\ -\langle\nabla\theta\rangle \\ -\langle\theta\rangle \end{bmatrix} \qquad \text{where} \qquad \langle\boldsymbol{f}\rangle = \frac{1}{\Omega}\int_\Omega \boldsymbol{f}(\boldsymbol{x})\,d\Omega. \tag{6}$$

where the integrals are extended to the morphology volume. In general, a certain number N_g of grains is selected and a certain number N_m of random morphologies with N_g grains are generated: the apparent properties associated with N_g grains are then computed as ensemble averages over the N_m realisations of the volume averages computed over each realisation with N_g grains. Further details about the overall procedure are given by Benedetti (2023).

3. Preliminary numerical tests

In this work preliminary results about thermo-elastic homogenisation of polycrystalline materials are presented, while micro-cracking simulations and results will form the core of forthcoming studies. Here the thermo-elastic ho-

mogenisation of silicon carbide at room temperature is addressed. Single crystal properties are taken as in Benedetti (2023) and Fig.(2) shows the results obtained from the described statistical homogenisation process for selected thermal conductivity and thermo-elastic constants: the homogenisation procedure produces results within the reference Reuss' and Voigt's bounds.

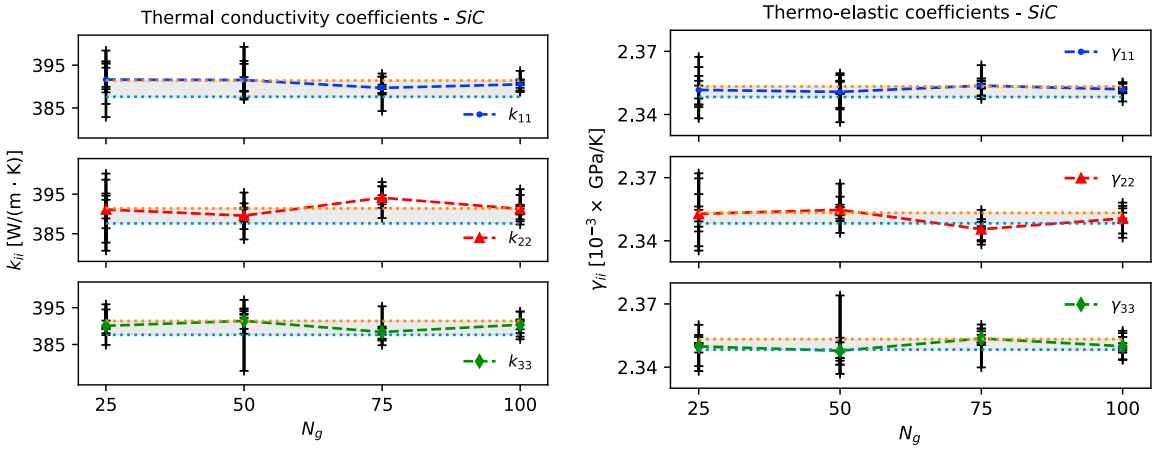

Fig. 2: Computational homogenisation results for selected components of thermal conductivity coefficients (*left*) and thermo-elastic coefficients (*right*) for polycrystalline silicon carbide. The '+' markers identify volume averages over single realisations, the dashed curves correspond to ensemble averages, while the shaded area lies between the Reuss' and Voigt's bounds.

4. Conclusions

The development of a boundary element framework for micro-thermo-mechanical analysis of polycrystalline materials has been presented. The framework key items have been described and it has been discussed how the developed tool can address both thermo-elastic homogenisation and micro-cracking of polycrystalline morphologies. It has been shown how the problem can be formulated in terms of pure boundary integral equations, in which the primary variables are nodal values of displacements, temperature jumps, tractions and thermal fluxes. The use of boundary integral equations allows a remarkable simplification of the meshing procedures, a consequent reduction in the number of degrees of freedom, and the direct employment of the boundary primary variables in the generalised cohesive laws used to model micro-cracking initiation and propagation. Results about thermo-elastic homogenisation of silicon carbide have been presented, showing how the proposed computational statistical homogenisation almost immediately converges to values of the thermo-elastic constants within the first order Voigt and Reuss bounds. Micro-cracking simulations will be presented in forthcoming studies.

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