A cohesive boundary element approach to material degradation in three-dimensional polycrystalline aggregates

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Abstract. A new three-dimensional grain-level formulation for intergranular degradation and failure in polycrystalline materials is presented. The polycrystalline microstructure is represented as a Voronoi tessellation and the boundary element method is used to express the elastic problem for each crystal of the aggregate. The continuity of the aggregate is enforced through suitable conditions at the intergranular interfaces. The grain-boundary model takes into account the onset and evolution of damage by means of an irreversible linear cohesive law, able to address mixed-mode failure conditions. Upon interface failure, a non-linear frictional contact analysis is introduced for addressing the contact between micro-crack surfaces. An incremental-iterative algorithm is used for tracking the micro-degradation and cracking evolution. The behavior of a polycrystalline specimen under tensile load has been performed, to show the capability of the formulation.

Introduction

For modern structural applications (aerospace, automotive, off-shore, etc.), a deep understanding of materials degradation and failure is of crucial relevance. Fracture modelling can be considered at different length scales: it is nowadays widely recognized that the macroscopic material properties depend on the features of the microstructure [1].

Polycrystalline materials (metals, alloys or ceramics) are commonly employed in engineering structures. Their microstructure is characterized by features of the grains (morphology, size distribution, anisotropy and crystallographic orientation, stiffness and toughness mismatch) and by physical and chemical properties of the intergranular interfaces. These aspects have a direct influence on the initiation and evolution of microstructural damage, which is also sensitive to the presence of imperfections, flaws or porosity.

The microstructure of polycrystalline materials, and its failure mechanisms, can be investigated using different experimental techniques (see references in [2] for a brief overview); these provide fundamental information and understanding but require sophisticated equipment, careful material manufacturing and preparation and complicated postprocessing, especially whenever a truly three-dimensional (3D) characterization is pursued.

A viable alternative, or complement, to the experimental effort is offered by the *Computational Micromechanics* [3]. Several investigations have been devoted to modelling of polycrystalline microstructures and their failure processes [4] and there is currently an interest for the development of truly 3D models. Until recently, this has been hindered by excessive computational requirements. However, the present-day availability of cheaper and more powerful computational resources and facilities, namely high performance parallel computing, is favoring the advancement of the subject, especially in the framework of the Finite Element Method (FEM), see e.g. [5].

A popular approach for modelling both 2D and 3D fracture problems in polycrystalline materials consists in the use of *cohesive surfaces* embedded in a finite element (FE) representation of the microstructure. In this way, initiation, propagation, branching and coalescence of microcracks stem as an outcome of the simulation, without any assumptions. Several cohesive laws have been proposed in the literature [6].

An alternative to the FEM is the Boundary Element Method (BEM) that has proved effective for a variety of physical and engineering problems [7,8]. A cohesive boundary element formulation for brittle intergranular failure in polycrystalline materials was proposed by Sfantos and Aliabadi [9]. A 3D grain boundary formulation has been recently developed by Benedetti and Aliabadi for the material homogenization of polycrystalline materials [2].

In this work, a novel 3D grain-level model for the analysis of intergranular degradation and failure in polycrystalline materials is presented. The polycrystalline microstructure is represented as a Voronoi tessellation and the formulation is based on a grain-boundary integral representation of the elastic problem for the anisotropic crystals, that have random orientation in the 3D space. The integrity of the aggregate is restored by enforcing suitable intergranular conditions. The onset and evolution of damage at the grain boundaries is modeled using an irreversible cohesive linear law. Upon interface failure, a non-linear frictional contact analysis is used, to address separation, sliding or sticking between micro-crack surfaces. An incremental-iterative algorithm is used for tracking the degradation and micro-cracking evolution. A numerical test is presented to demonstrate the capability of the formulation.

Grain boundary formulation for polycrystalline aggregates

Artificial microstructure. For polycrystalline materials, Voronoi tesselations are widely used for the generation of the microstructural models [10]. The assignation of a specific orientation to each crystal of the aggregate completes the microstructure representation.

Grain constitutive modelling. Each grain is modeled as a three-dimensional linear elastic orthotropic domain with arbitrary spatial orientation. This is not restrictive, as the majority of single metallic and ceramic crystals present general orthotropic behavior.

Grain boundary element formulation. Each crystal is modeled using the BEM for 3D anisotropic elasticity [11]. The polycrystalline aggregate is seen as a multi-region problem, so that different elastic properties and spatial orientation can be assigned to each grain [2]. Given a volume bounded by an external surface and containing N_g grains, two kinds of grains can be distinguished: the *boundary grains*, intersecting the external boundary, and the *internal grains*, completely surrounded by other grains. Boundary conditions are prescribed on the surface of the boundary grains lying on the external boundary, while interface equations and equilibrium conditions are forced on interfaces between adjacent grains, to restore the integrity of the aggregate. The boundary integral equation for a generic grain $\mathcal{G}_k$ is written

$$\tilde{c}_{ij}^{k}\left(\boldsymbol{x}\right)\tilde{u}_{j}^{k}\left(\boldsymbol{x}\right)+\int_{B_C\cup B_{NC}}\tilde{T}_{ij}^{k}\left(\boldsymbol{x},\boldsymbol{y}\right)\tilde{u}_{j}^{k}\left(\boldsymbol{y}\right)dB^{k}\left(\boldsymbol{y}\right)=\int_{B_C\cup B_{NC}}\tilde{U}_{ij}^{k}\left(\boldsymbol{x},\boldsymbol{y}\right)\tilde{t}_{j}^{k}\left(\boldsymbol{y}\right)dB^{k}\left(\boldsymbol{y}\right) \tag{1}$$

where $\tilde{u}_j^k$ and $\tilde{t}_j^k$ represent components of displacements and tractions of points belonging to the surface of the grain $\mathcal{G}_k$, the tilde refers to quantities expressed in a local reference system set on the grain surface, $\tilde{U}_{ij}^k$ and $\tilde{T}_{ij}^k$ are the 3D displacement and traction fundamental solutions for the anisotropic elastic problem.

The integrals in Eq.(1) are defined over the surface of the grain, that is generally given by the union of *contact* interfaces B_C and external *non-contact* surfaces B_{NC}. The model for the polycrystalline aggregate is obtained by writing Eq.(1) for each grain and then complementing the system so obtained with the *boundary conditions*

$$\tilde{u}_i=\overline{u}_i \quad or \quad \tilde{t}_i=\overline{t}_i \quad on\ B_{NC} \tag{2}$$

and with a set of suitable *interface equations*, expressing the different possible states of an interface.

Interface model. The interface between two grains can be in three different possible states: *pristine*, when no damage is present and perfect bonding between the grains holds; *damaged*, when damage is present and intergranular tractions and displacement jumps are linked through a cohesive traction-separation law; *failed*, when the grains are completely separated and the laws of the frictional contract mechanics hold.

Let us consider two adjacent grains $\mathcal{G}_a$ and $\mathcal{G}_b$. When the interface between them is in pristine state, the following interface continuity equations hold

$$\delta\tilde{u}_i^{ab} = \tilde{u}_i^a + \tilde{u}_i^b = 0 \quad (\textit{continuity}) \qquad \textit{and} \qquad \tilde{t}_i^a = \tilde{t}_{ii}^b \quad (\textit{equilibrium}) \tag{3}$$

The previous equations express the absence of interface displacement opening and the equilibrium of the interface tractions. The equilibrium equations always hold during the analysis, regardless the interface state, so they are always assumed in the following, while the continuity equations are replaced by other laws expressing the interface state during the interface evolution.
Damage is introduced at the interface when the value of a suitable *effective traction* overcomes the *interface cohesive strength* $T_{\max}$

$$t_{eff} = \left[\left\langle \tilde{t}_n \right\rangle^2 + \left(\frac{\beta}{\alpha} \tilde{t}_t \right)^2 \right]^{\frac{1}{2}} \geq T_{\max} \tag{4}$$

In the previous equation, the local tractions are expressed in terms of local normal and tangential contribution, $\tilde{t}_n$ and $\tilde{t}_t$. The parameters α and β give different weight to mode I and mode II loading. When the previous condition is fulfilled, the following traction-separation laws are introduced at the interface

$$\begin{bmatrix} \tilde{t}_1 \\ \tilde{t}_2 \\ \tilde{t}_3 \end{bmatrix} = T_{\max} \frac{1-d^*}{d^*} \begin{bmatrix} \alpha / \delta u_t^c & 0 & 0 \\ 0 & \alpha / \delta u_t^c & 0 \\ 0 & 0 & 1 / \delta u_n^c \end{bmatrix} \begin{bmatrix} \delta\tilde{u}_1 \\ \delta\tilde{u}_2 \\ \delta\tilde{u}_3 \end{bmatrix} \tag{5}$$

where $d^* \in [0,1]$ is a damage parameter given by

$$d^* = \max_{\textit{Loading history}} \{d\} \qquad \textit{with} \qquad d = \left[\left\langle \frac{\delta u_n}{\delta u_n^c} \right\rangle^2 + \beta^2 \left(\frac{\delta u_t}{\delta u_t^c} \right)^2 \right]^{\frac{1}{2}} \tag{6}$$

where δu_n and δu_t are the normal and tangential opening displacements at the interface and δu_n^c and δu_t^c represent their critical values in pure mode I and II respectively. The parameter *d* is the *effective opening displacement* and the damage parameter is given by the maximum value reached by the effective displacement during the loading history. For $d^* = 0$ the interface is pristine, while $d^* = 1$ expresses the failure of the interface.
Upon interface failure, the traction-separation laws are replaced by the laws of the *frictional contact mechanics*. In general, the micro-crack surfaces can be either *separated* or in *contact*; moreover, two surfaces in contact can either *stick* or *slip* over each other. The equations of frictional contact mechanics are not recalled here, but the interested reader is referred to the literature on the subject (see [8] and references therein).

Discretization and numerical solution. The present formulation has the advantage that only meshing of the grain surfaces is required. The artificial microstructure is, in this context, a collection of flat convex polygonal faces. Plane triangular linear elements are used to discretize such faces. Linear discontinuous triangular elements are implemented for representing the unknown boundary fields. Since the Voronoi tessellations used for microstructure modelling have stochastic nature, care must be taken to ensure mesh consistency and homogeneity to the greatest extent [2].

After discretization and classical BEM treatment of the Eqs.(1), the following system can be written

$$\begin{bmatrix} \mathbf{A}_1 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \ddots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{A}_{N_g} \\ [& \boldsymbol{\Psi}(d^*) &] \end{bmatrix} \begin{bmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_{N_g} \end{bmatrix} = \begin{bmatrix} \mathbf{y}_1 \\ \vdots \\ \mathbf{y}_{N_g} \\ \boldsymbol{\psi} \end{bmatrix} \tag{7}$$

where the matrix blocks $\mathbf{A}_k$ contain columns of the boundary element matrices $\mathbf{H}_k$ and $\mathbf{G}_k$ corresponding to the unknown displacements and tractions of the *k-th* grain, contained in the vector $\mathbf{x}_k$, and $\mathbf{y}_k$ derive

from the applications of the known boundary conditions. The block $\mathbf{\Psi}\left(d^*\right)$ implements the varying coefficients of the interface equations, i.e. the continuity, cohesive and frictional contact equations, for all the grain boundary interfaces.

System (7) is sparse and special solvers can be used for its solution. To track the evolution o f a poly-crystalline microstructure, an *incremental/iterative algorithm* is employed. A load increment is applied and the system solution is iterated until no violation of the interface equations is detected. At each iteration, all the interfaces are checked, to assess whether any violation of the assumed interface state is detected. For example, if the effective traction of a pristine interface overcomes the cohesive strength, then damage is initiated and the continuity equations are replaced by cohesive laws. Analogous checks are also done for interfaces in the cohesive or failed state. For the damaged interfaces, the cohesive law has to be updated if a loading condition exists, while no update is required in the cases of unloading or reloading. When convergence is reached a new load increment can be applied and the iterative search is restarted.

In this work PARDISO [12] is used as iterative solver and a hybrid direct/iterative solution strategy is employed to speed up the numerical solution of the polycrystalline evolution problem.

Numerical simulation of a SiC micro-specimen under tensile load

A prismatic polycrystalline specimen subjected to tensile load is considered. The specimen is comprised of $N_g = 200$ fully three-dimensional *SiC* grains; an uniform displacement is applied over the bases and it is directed along the longer side, Fig.1. The material properties for crystalline *SiC* are given in Table **1**, the grain size is ASTM G=12 (calculated number of grains per mm^3: $n/v = 4.527 \cdot 10^6$ [13]). The specimen's size is $2W \times 2W \times 2H$ with $H/W = 2$, its volume is $V = 8HW^2 = N_g \cdot \bar{V}_{grain}$, where $\bar{V}_{grain}$ is the estimated average grain volume. The mesh density is specified by $d_m = 0.5$ (see [2] for further details about the meshing strategy). The properties of the interfaces are uniform and they are given in Table **2**.

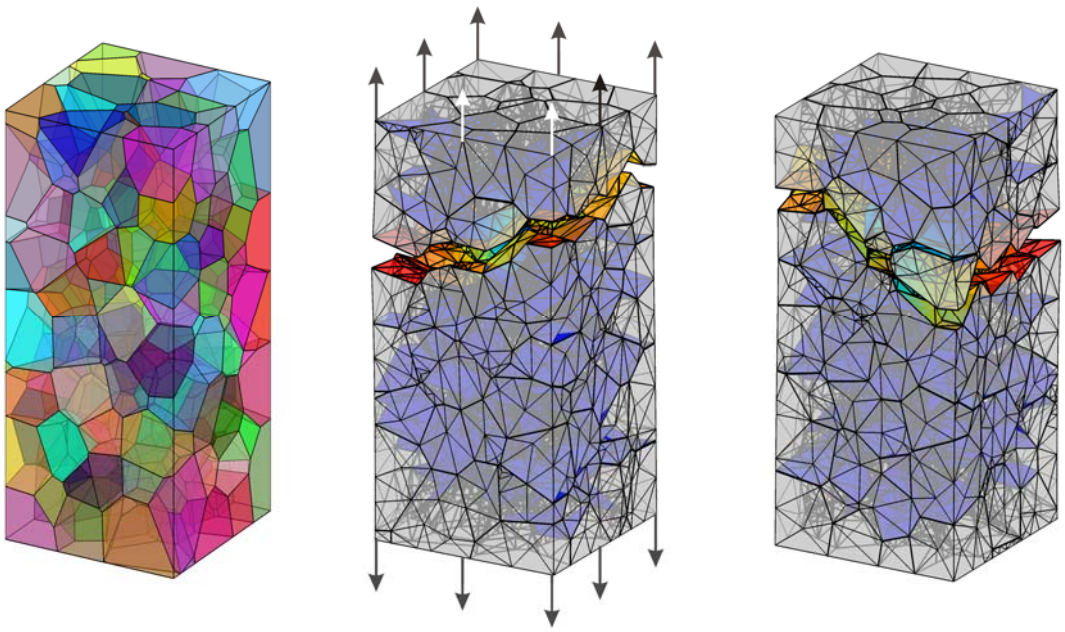

Figure 1: Polycrystalline *SiC* specimen with 200 grains subjected to tensile load.

C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}
502	95	96	565	169	203.5

Table 1: Material constant for single SiC crystals.

Fig. 1 shows the microstructural crack pattern immediately before the complete failure of the specimen. The corresponding macroscopic stress-strain curve is shown in Fig.2. The curve reports the value of the relevant component of the averaged stress tensor versus the nominal strain, obtained from the value of the applied displacement over the relevant specimen size. It is apparent how the specimen softens before the complete failure. Table 3 reports some statistics about the considered microstructure.

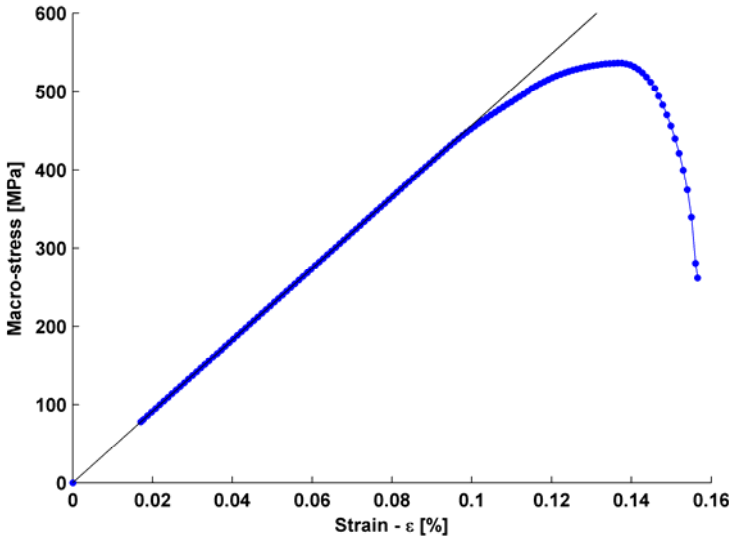

Figure 2: Volume average stress component versus nominal strain for the considered specimen.

$T_{\max}$	α	β	G_{II}/G_I	μ
500	1	$\sqrt{2}$	1	0.05

Table 2: Selected values for the interface properties.

$N_{elements}$	$N_{interfaces}$	DoFs	$T_{\Delta\lambda}$
17,031	7,709	222,660	~5000s

Table 3: Some statistics about the considered polycrystalline specimen.
The time per load increment was measured on 12-core nodes.

Summary

A new three-dimensional formulation for the analysis of intergranular degradation and failure in polycrystalline materials has been developed. The polycrystalline microstructure is represented as a three-dimensional Voronoi tessellation, able to retain the main morphological and crystallographic features of polycrystalline aggregates. The micromechanical model is expressed in terms of intergranular fields, namely displacement jumps and tractions. The nucleation and evolution of intergranular damage has been followed using an irreversible cohesive law at the intergranular interfaces: this resulted particularly straightforward, being the formulation itself expressed in terms of grain boundary variables. Upon complete intergranular failure the frictional contact analysis is introduced to follow the intergranular micro-cracking process, taking into account separation, contact and sliding between the micro-crack surfaces.
A numerical test demonstrated the capability of the formulation to model the nucleation, evolution and coalescence of multiple damage and cracks. For its nature, the developed formulation appears particularly promising in the framework of *grain boundary engineering*.

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