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A Novel Micro-Mechanical Model for Polycrystalline Inter-Granular and Trans-Granular Fracture

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Abstract. In this work, a novel grain boundary formulation for inter- and trans-granular cracking of polycrystalline materials is presented. The formulation is based on the use of boundary integral equations for anisotropic solids and has the advantage of expressing the considered problem in terms of grain boundary variables only. Inter-granular cracking occurs at the grain boundaries whereas trans-granular cracking is assumed to take place along specific cleavage planes, whose orientation depends on the crystallographic orientation of the grains. The evolution of inter- and trans-granular cracks is then governed by suitably defined cohesive laws, whose parameters characterize the behavior of the two fracture mechanisms. The results show that the model is able to capture the competition between inter- and trans-granular cracking.

Introduction

Recent advances in microscopy and high performance computing have motivated much research on the study of materials at nano- and microscopic scales. In such a context, the affordability of more powerful computational tools and facilities has allowed the inclusion, in various models, of microstructural details of ever increasing complexity. The study of polycrystalline materials, which include most metals and ceramics, exemplifies the trend sketched above. Polycrystalline materials have been intensely investigated and an increasing level of realism is being achieved in their virtual modeling.

In this framework, we propose a grain-boundary model for inter- and trans-granular micro-cracking in 3D polycrystalline morphologies. The model is based on the use of a multi-region boundary integral representation of the aggregate mechanics [2,3,4,5,6], in conjunction with a cohesive zone approach, which is used for representing both inter- and trans-granular degradation and cracking. Trans-granular cracks are introduced into the grains when a suitably defined stress threshold condition is fulfilled. The conditions for the activation of trans-granular cleavage processes are discussed and a numerical investigation on the effects of the cohesive materials parameters on the interplay between inter- and trans-granular failures is performed. A distinguishing feature of the model is that all the relevant mechanical fields are represented in terms of grain-boundary variables only, which simplifies data preparation and re-meshing and reduces the overall number of DoFs with respect to other popular techniques.

Formulation

The presented formulation is based on the use of a multi-region boundary integral approach for anisotropic solids [1,2,3]. To model inter- and trans-granular cracking in polycrystalline materials, the displacement boundary integral equations (DBIEs) and the stress boundary integral equations (SBIEs) are used during the analysis [1]. Each grain within the aggregate is modelled as an anisotropic elastic domain with random spatial orientation. Its constitutive behavior is expressed by

$\sigma_{ij} = C_{ijkl}\varepsilon_{kl}$ where σ_{ij}, ε_{ij} and C_{ijkl} are the components of the stress, strain and elasticity tensors. In this framework, the DBIEs read

$$c_{ij}(\mathbf{y})u_j(\mathbf{y}) + \int_S T_{ij}(\mathbf{x},\mathbf{y})u_j(\mathbf{x})dS(\mathbf{x}) = \int_S U_{ij}(\mathbf{x},\mathbf{y})t_j(\mathbf{x})dS(\mathbf{x}), \quad (1)$$

where u_i and t_i are the grain boundary displacements and tractions; T_{ij} and U_{ij} are the fundamental solutions for 3D anisotropic elasticity, **x** is the boundary integration point, **y** is the collocation point and c_{ij} are the free-terms stemming from the boundary limiting process.

The SBIEs, at an internal point **y**, are written as

$$\sigma_{ij}(\mathbf{y}) + \int_S S_{ijk}(\mathbf{x},\mathbf{y})u_k(\mathbf{x})dS(\mathbf{x}) = \int_S D_{ijk}(\mathbf{x},\mathbf{y})t_k(\mathbf{x})dS(\mathbf{x}) \quad (2)$$

where S_{ijk} and D_{ijk} are derived from the fundamental solutions in Eq.(1) [1,8].

The polycrystalline problem is closed by means of a properly defined set of boundary and interface conditions. The boundary conditions (BCs) are enforced on the external faces of the aggregate by prescribing the values of the displacements and/or tractions. The interface conditions (ICs) are enforced on the boundaries shared by two contiguous grains and, as long as the generic interface is intact, are defined by displacements continuity and tractions equilibrium. The reader is referred to [2,4] for further details on the used modelling strategy.

Inter- and trans-granular cracking model

Inter- and trans-granular cracks are modelled with cohesive laws [2,6]. Damage is assumed to arise over either inter- or trans-granular interfaces when a suitably defined *effective traction* overcomes the *interface strength*. When the threshold criterion is fulfilled, a cohesive law of the form $\tilde{t}_i = K_{ij}(d^*)\delta\tilde{u}_j$ is introduced to link the boundary traction components $\tilde{t}_i$ with the displacements jump $\delta\tilde{u}_i$ expressed in the grain boundary local reference system. The cohesive law is given in terms of the constants $K_{ij}(d^*)$, which are function of the irreversible damage parameter d^* that in turn is defined in terms of an effective opening displacement [2,5].

Although inter- and trans-granular processes are modelled using an analogous cohesive approach, it is worth underlining their different nature and numerical treatment. Inter-granular failures occur along the interfaces between adjacent grains, which are naturally defined within the original polycrystalline morphology. On the other hand, at a generic point within the bulk crystallographic lattice of a crystal, trans-granular failure may potentially occur along different planes, which are not *a priori* known and may or may not activate depending on the fulfilment of a threshold cleavage condition. Consequently, trans-granular cracks are introduced dynamically during the analysis as soon as the cleavage stress overcomes the strength of the potential cleavage planes.

Moreover, the evolution of inter- and trans-granular cracking is governed by two different cohesive laws, whose parameters are set to represent the different properties of the two types of interfaces. The interplay between the two mechanisms is governed by a parameter γ_G that expresses the ratio between the energies of separation of inter- and trans-granular cracking and it is defined as $\gamma_G = G_I^g / G_I^{gh}$, where G_I^g and G_I^{gh} denote the work of separation in pure normal mode characterizing trans- and inter-granular cracking, respectively. The work of separation G_I, the interface strength $T_{\max}$, the ratio G_I/G_{II}, where G_{II} is the work of separation in pure sliding mode and two parameters weighing the normal and sliding modes are subsequently used to define the constants entering each cohesive law [2,5].

Numerical discretization and solution algorithm

The solution of the 3D polycrystalline problem with inter- and trans-granular cracking is obtained by discretizing Eqs.(1-2) according to the strategy developed in [7].
The equations of the whole aggregate are retrieved by discretizing Eq.(1) for each grain and by using the suitable boundary and interface equations [5,7]. A non-linear system of equations of the form $\mathbf{M}(\mathbf{X},\lambda)=\mathbf{0}$ is obtained, where $\mathbf{X}$ contains the unknown values of displacements and tractions and λ is the load factor [5,7].
During the generic load step, Eq.(2) is used to compute the components of the stress tensor at the selected control points. If the trans-granular threshold condition is fulfilled, an activated trans-granular cleavage plane is introduced and a re-meshing of the aggregate is performed. Then, the solution with the *new* morphology is computed for the *same* load factor.

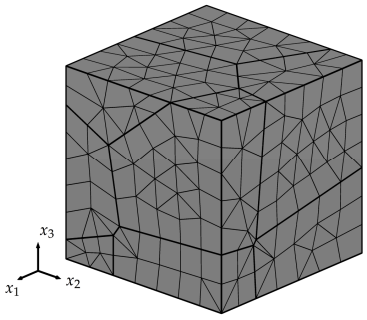
Numerical tests

In this section, the cracking behavior of a polycrystalline SiC 10-grain morphology with ASTM grain size G = 12 is tested. For hexagonal 6H SiC polytypes, the preferred cleavage plane is the basal plane [9] identified by the (0001) Miller indices. The non-zero elastic constants in the grain local reference system are C_{1111} = C_{2222} = 502 GPa, C_{3333} = 565 GPa, C_{1122} = 95 GPa, C_{1133} = C_{2233} = 96 GPa, C_{2323} = C_{1313} = 169 GPa, C_{1212} = (C_{1111}-C_{1122})/2. The non-zero constants of the inter-granular cohesive law are

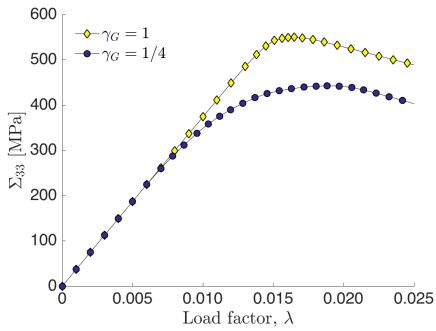
$$K_{11}(d^*)=K_{22}(d^*)=\alpha\frac{T_{\max}}{\delta u_s^{cr}}\frac{1-d^*}{d^*}\quad and\quad K_{33}(d^*)=\frac{T_{\max}}{\delta u_n^{cr}}\frac{1-d^*}{d^*}, \tag{3}$$

whose parameters are $T_{\max}=500\text{MPa}$, $\delta u_n^{cr,gh}=7.80\cdot10^{-2}$, $\delta u_s^{cr,gh}=1.56\cdot10^{-1}$, $\alpha^{gh}=1$. To enforce the ratio $\gamma_G=G_I^g/G_I^{gh}$, the parameters of the trans-granular cohesive law are $T_{\max}^g=\sqrt{\gamma_G}\cdot T_{\max}^{gh}$, $\delta u_n^{cr,g}=\sqrt{\gamma_G}\cdot\delta u_n^{cr,gh}$, $\delta u_s^{cr,g}=\sqrt{\gamma_G}\cdot\delta u_s^{cr,gh}$, $\alpha^{gh}=\alpha^g$.

The morphology and its mesh is shown in Fig.(1a). The aggregate is subject to prescribed macro-strain Γ_{33} along the x_3 direction. Two values of γ_G are considered, namely $\gamma_G=1$ and $\gamma_G=1/4$. The curves showing the macro-stress Σ_{33} as a function of the load factor for the two values of γ_G are given in Fig.(1b). Fig.(2) show the crack pattern at the last computed step for $\gamma_G=1$ and $\gamma_G=1/4$, respectively. In Fig.(2a), although one grain gets cut during the analysis, the fracture is predominantly inter-granular, whereas, in Fig.(2b), it is possible to see that reducing the trans-granular fracture energy favors the trans-granular mechanism itself.

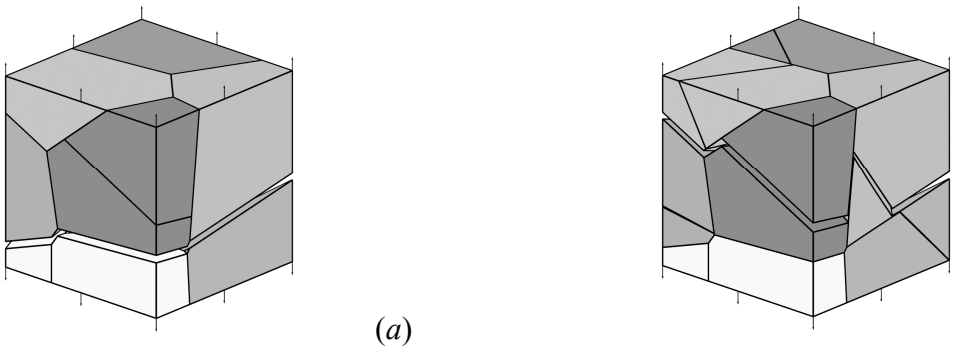


(*a*)



(*b*)

Fig. 1: *a*) Grain boundary mesh of a 10-grain polycrystalline morphology with ASTM grain size G = 12; *b*) Volume stress average Σ_{33} as a function of the load factor λ for the two considered values of the ratio γ_G between the inter- and trans-granular fracture toughness.



(*a*) (*b*)

Fig. 2: Crack patterns at the last computed step of the considered morphology for the two values of the ratio γ_G between the inter- and trans-granular fracture toughness: *a*) $\gamma_G = 1$ *b*) $\gamma_G = 1/4$.

Summary

In this study, a novel numerical scheme for addressing the competition between inter- and trans-granular crack propagation has been developed and tested. The formulation is based on a grain boundary formulation for polycrystalline micro-mechanics and expresses the polycrystalline problems in terms of grain boundary variables only. Trans-granular failures are modelled by suitably oriented trans-granular cracks introduced upon the fulfillment of a threshold cleavage condition.
Results show that the method captures the behavior of polycrystalline aggregates when the two mechanisms are active. Future work will involve morphologies with larger numbers of grains and the coupling with other polycrystalline deformation mechanisms such as crystal plasticity [10].

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