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A three-dimensional cohesive-frictional grain-boundary micromechanical model for intergranular degradation and failure in polycrystalline materials

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ABSTRACT

In this study, a novel three-dimensional micro-mechanical crystal-level model for the analysis of intergranular degradation and failure in polycrystalline materials is presented. The polycrystalline microstructures are generated as Voronoi tessellations, that are able to retain the main statistical features of polycrystalline aggregates. The formulation is based on a grain-boundary integral representation of the elastic problem for the aggregate crystals, that are modeled as three-dimensional anisotropic elastic domains with random orientation in the three-dimensional space. The boundary integral representation involves only intergranular variables, namely interface displacement discontinuities and interface tractions, that play an important role in the micromechanics of polycrystals. The integrity of the aggregate is restored by enforcing suitable interface conditions, at the interface between adjacent grains. The onset and evolution of damage at the grain boundaries is modeled using an extrinsic non-potential irreversible cohesive linear law, able to address mixed-mode failure conditions. The derivation of the traction-separation law and its relation with potential-based laws is discussed. Upon interface failure, a non-linear frictional contact analysis is used, to address separation, sliding or sticking between micro-crack surfaces. To avoid a sudden transition between cohesive and contact laws, when interface failure happens under compressive loading conditions, the concept of cohesive-frictional law is introduced, to model the smooth onset of friction during the mode II decohesion process. The incremental-iterative algorithm for tracking the degradation and micro-cracking evolution is presented and discussed. Several numerical tests on pseudo- and fully three-dimensional polycrystalline microstructures have been performed. The influence of several intergranular parameters, such as cohesive strength, fracture toughness and friction, on the microcracking patterns and on the aggregate response of the polycrystals has been analyzed. The tests have demonstrated the capability of the formulation to track the nucleation, evolution and coalescence of multiple damage and cracks, under either tensile or compressive loads.

1. Introduction

The development of critical structures requires deep understanding of mechanisms governing degradation and failure of materials, especially when applications in severe environments are considered. Fracture modeling can be considered at different length scales: it is nowadays widely recognized that macroscopic material properties depend on the features of the microstructure. The knowledge of this link, which is the main subject of *Micromechanics* [1–3], is of relevant technological interest, as it may enable the design of materials with specific requirements in terms of strength, stiffness, ductility, toughness, etc., by means of suitable manipulations of the microstructural features that have a desired effect on the sought macroscopic property.

Polycrystalline materials, either metals, alloys or ceramics, are commonly employed in practical structures. Their microstructure, generally in the range from 10^{-6} to 10^{-3} m, is characterized by features of the grains, their morphology, size distribution, anisotropy and crystallographic orientation, stiffness and toughness mismatch, and by physical and chemical properties of the intergranular interfaces [4]. All these aspects have a direct influence on the initiation and evolution of the microstructural damage, which is also sensitive to the presence of imperfections, flaws or porosity. Any theory or model for explaining failure mechanisms in this class of materials must then accommodate a relevant number of parameters [5].

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Depending on a specific material and load and environment conditions, polycrystalline materials exhibit different failure mechanisms spanning from ductile to brittle fracture. Brittle failure, moreover, can be related to two main microstructural mechanisms, i.e. cleavage or transgranular fracture, in which the crack propagates on specific crystallographic planes *within* the grains, and intergranular failure, in which the microcracks follow the grain boundaries.

Brittle intergranular failure may occur in metals, alloys and ceramics [6] and it is particularly dependent on the chemical-physical state of the grains interfaces [7–9], namely on the segregation of impurities and/or embrittling particles or on the presence of precipitate-free zones, in the case of precipitation-strengthened materials, [10–18]. Intergranular failure is also favored by hostile environmental conditions [19], by phenomena such as corrosion [20] or stress-corrosion cracking [21,22] or by some combination of stress and high temperature [23]. The investigation and modeling of the brittle intergranular failure is then particularly relevant for better understanding and design with polycrystalline materials: in this framework it is worth noting that the concept of *grain boundary engineering* is now well established [24].

The microstructure of polycrystalline materials, and its influence on the microscopic failure mechanisms and on macroscopic material behavior, can be investigated by using different experimental techniques [25–33]. The experimental techniques for materials reconstruction and characterization are necessary for providing fundamental information and understanding; however, they require sophisticated equipment, careful material manufacturing and preparation, complicated postprocessing. They are generally expensive and time consuming. Such aspects are relevant whenever a truly three-dimensional (3D) characterization is pursued, or the simultaneous effect of several microstructural features is studied, or damage and failure at the microstructural level are investigated.

A viable alternative, or complement, to the experimental effort is offered by *computational micromechanics*. Several investigations have been devoted development of numerical models for the analysis of polycrystalline microstructures and their failure processes, both in two and three dimensions [5]: among different approaches, multiscale methods appear to be the most promising, as they are able to bring together and link the diverse scales acting in the initiation and evolution of fracture [34–38].

Several techniques have been developed and used for studying the crack initiation and propagation in heterogeneous or polycrystalline microstructures. Kamaya [39] employed the body force method for investigating 2D intergranular stress corrosion cracking. Sukumar et al. [40] studied the competition between inter- and transgranular crack growth in 2D polycrystalline brittle microstructure by using the extended FEM. Das et al. [41] coupled finite elements and cellular automata (CAFE) and showed the potential for microstructural and multiscale analysis of heterogeneous and polycrystalline materials. Also lattice models for quantitative estimates of the mechanical properties of polycrystalline microstructures and their damage have been reported [42]. The application and advantages of peridynamics for modeling crack initiation, propagation and fragmentation in polycrystalline ceramics are discussed in [36].

The above studies have mainly focused on the analysis of 2D polycrystalline problems, although some 3D applications of cellular automata and finite elements have been reported and the 3D potential of peridynamics has been discussed. There is currently an interest for development of truly 3D models for analysis of failure mechanisms in polycrystalline materials [5,43–45]. This is motivated, on one hand, by the need for understanding complex inherently 3D phenomena (such as the influence of the geometry on the microcracking evolution; the competition between different failure modes, e.g. inter- and transgranular brittle propagation or the ductile-to-brittle transition; the grain-to-grain propagation of cleavage fracture [46]) and, on the other hand, by the need of complementing experimental investigations that, in the case of 3D microstructure reconstruction and characterization are particularly complex and expensive, especially when damage and failure are considered. Until recently, development of truly 3D models has been hindered by their 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 [47–50].

A 3D rigid bodies-spring model for the analysis of brittle microcracking in polycrystalline Voronoi microstructures was developed by Toi and Kiyosue [51]. Marrow et al. [44] developed a simple 3D model for the analysis of intergranular stress corrosion cracking in austenitic stainless steel: in order to reduce the computational effort, in their model each grain is represented by a discrete system of elasto-plastic beams; grain boundaries are classified as either susceptible or resistant to intergranular fracture and different simplified failure criteria are assumed for them. Hughes et al. [45] developed a 3D geometrical model of the brittle fracture in polycrystalline zinc, with a focus on propagation of cleavage cracks from grain to grain. The stress corrosion intergranular crack initiation and growth in 3D polycrystalline microstructures was studied by using the finite element analysis by Kamaya and Itakura [52]. In their work the initiation and propagation of the cracks were modeled applying the concepts of damage mechanics. Musienko and Cailletaud [53] simulated inter- and transgranular stress corrosion cracking in polycrystalline aggregates with a finite element model in which the single grains exhibit viscoplastic behavior, transgranular cleavage is accommodated by introducing a pseudo-strain in the crystal plasticity framework and the grain boundaries are modeled as thin viscoplastic finite elements modified in the spirit of damage mechanics. Finite elements and continuum damage mechanics have been combined by Bomidi et al. for modeling of intergranular fatigue failure of 3D fine grain polycrystalline metallic MEMS devices [50].

A popular approach for modeling 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. The cohesive zone models provide a phenomenological framework in which the complex physical phenomena underlying the initiation and evolution of damage, in the so called process zone, are embedded in a traction-separation law expressing the progressive loss of material cohesion. In this way, initiation, propagation, branching and coalescence of microcracks stem as an outcome of the simulation, without any *a priori* assumptions. Several cohesive laws have been proposed [54,55], but most popular are the potential-based laws by Tvergaard [56] and Xu and Needleman [57] and the linear laws by Camacho and Ortiz [58] and Ortiz and Pandolfi [59].

Cohesive FE models for 2D microstructures have been presented by several authors. Zhai and Zhou [60,61] used the cohesive FE method for studying the quasi-static and dynamic failure in heterogeneous two-phase Al_2O_3/TiB_2 ceramic microstructures. Espinosa and Zavattieri [62,63] developed a grain level model for the analysis of intergranular failure initiation and evolution in brittle polycrystalline materials and discussed the features of different cohesive laws in numerical simulations. Wei and Anand [64] employed crystal plasticity theory and cohesive laws in a FE framework to study the dominant failure mechanisms in nanocrystalline fcc metals and carried out simulations on pseudo-3D microstructures (columnar grains). The dynamic fragmentation of granular ceramic microstructures has been studied with a cohesive FE scheme by Maiti et al. [65]. Zhou et al. [66] simulated crack growth in the