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Multiscale modeling of polycrystalline materials: A boundary element approach to material degradation and fracture

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Highlights

- A two-scale 3D framework for polycrystalline degradation and failure is proposed.
- The macroscale is modeled using a 3D boundary element initial stress approach.
- The microscale is modeled using a 3D grain-boundary cohesive-frictional model.
- The macroscale provides periodic boundary conditions to the micro-RVEs.
- The micro-RVEs provide the macro-damage evolution to the macro-scale.

Abstract

In this work, a two-scale approach to degradation and failure in polycrystalline materials is proposed. The formulation involves the engineering component level (macro-scale) and the material grain level (micro-scale). The macro-continuum is modeled using a three-dimensional boundary element formulation in which the presence of damage is formulated through an *initial stress approach* to account for the local softening in the neighborhood of points experiencing degradation at the micro-scale. The microscopic degradation is explicitly modeled by associating Representative Volume Elements (RVEs) to relevant points of the macro continuum, for representing the polycrystalline microstructure in the neighborhood of the selected points. A three-dimensional grain-boundary formulation is used to simulate intergranular degradation and failure in the microstructure, whose morphology is generated using the Voronoi tessellations. Intergranular degradation and failure are modeled through cohesive and frictional contact laws. To couple the two scales, macro-strains are transferred to the RVEs as periodic boundary conditions, while overall macro-stresses are obtained as volume averages of the micro-stress field. The comparison between effective macro-stresses for the damaged and undamaged RVE allows to define a macroscopic measure of material degradation. To avoid pathological damage localization at the macro-scale, integral non-local counterparts of the strains are employed. A multiscale processing algorithm is described. Two multiscale simulations are performed to demonstrate the capability of the method.

Keywords: Polycrystalline materials; Damage and fracture; Multiscale formulations; Micromechanics; Boundary element method

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1. Introduction

The design of materials for advanced applications requires full understanding of the material response to different operational and environmental conditions and, often, the knowledge of their failure mechanisms is of great relevance. Phenomenological models at the component level may not always be able to predict complex materials behaviors, especially when initiation and evolution of damage are involved. It is widely recognized that such aspects may be better understood if the physical details of the material microstructure are brought into the modeling framework. The link between microstructure and material macroscopic properties, i.e. the *structure–property* relationship [1–4], is technologically interesting and it may provide valuable information for the design of enhanced high-performance materials [5].

Polycrystalline materials (metals, alloys or ceramics) are widely used in the engineering practice. Their microstructure, at the grain scale, is characterized by grains morphology, size distribution, anisotropy and crystallographic orientation, by the presence of flaws and porosity and by physical and chemical properties of the intergranular interfaces [6], which have direct influence on the initiation and evolution of damage.

Polycrystalline microstructures have been studied using experimental [7–15] and computational techniques [4,16, 17]. Much research has been carried out for developing numerical models for polycrystalline microstructures and their failure processes. Until recently, the development of truly three-dimensional (3D) models has been hindered by excessive computational requirements. In recent years, however, *computational micromechanics* has experienced a remarkable acceleration, due to the wider affordability of high performance parallel computing (HPC), thus favoring the advancement of the subject [18–21].

There are several scientific and technological reasons for the interest in truly 3D polycrystalline models [22–26]. Three-dimensional models allow better understanding of inherently 3D complex microstructural phenomena: 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 [27]; the plastic deformation of the individual crystals. Computational investigations complement experimental techniques that, in the 3D case, may be particularly complex and expensive, especially when damage and failure are considered. Moreover, an increasing number of applications, in different fields, require the manufacturing of micro-components whose overall dimensions are comparable with the grain size, thus requiring accurate analysis at the grain scale level. The direct simulations of polycrystalline microstructures, and their micro-damaging processes, find remarkable applications in the *multiscale analysis of materials and solids*, where a component is analyzed simultaneously at the *component level*, in which the load history is defined, and at the *grain scale level*, which provides the constitutive material evolution. The term multiscale may assume a variety of meanings [28–31]: however, here the focus is on simulations involving two spatial scales, the continuum level and the grain scale level, for which a clear *scale separation* holds. The objective is to analyze both the macro-component and the processes occurring in the microstructure, during the loading history. The multiscale analysis becomes particularly effective when, during the loading history, the microstructure undergoes phase transformations or damage, so that a simple constitutive model assumed at the macro-level could not be used to simulate the behavior of the structure.

It is worth mentioning that, due to the enormous computational effort required by a fully *three-dimensional* multiscale analysis, which usually involves the simultaneous solution of several three-dimensional non-linear microstructural problems, such analyses are quite rare in the literature. Several reviews on multiscale modeling of heterogeneous materials are available, see [32,33] and references therein. Geers et al. [32] analyzed recent trends and challenges in multiscale computational homogenization, briefly reviewing first-order techniques for mechanical problems, the concepts of second-order, continuous–discontinuous and multi-physics homogenization, applications to thin structures and problems involving interface and cohesive problems. A review on multiscale models for localization problems has been recently given by Nguyen et al. [33], who focused, among other topics, on continuous and discontinuous computational homogenization for adhesive/cohesive crack modeling and cohesive failures.

Multiscale models have been developed for the analysis of different classes of materials. Unger and Eckardt [34] developed a concurrent embedded multiscale method for studying the non-linear behavior of concrete structures, modeling explicitly the mortar matrix, the coarse aggregates and the interfacial transition zone at the material mesoscale and testing different methods (constraint equations, mortar method and arlequin method) for coupling the different length-scales.