Intergranular damage and fracture in polycrystalline materials.
A novel 3D microstructural grain-boundary formulation.

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The design of advanced materials requires a deep understanding of degradation and failure processes. It is widely recognized that the macroscopic material properties depend on the features of the microstructure. The knowledge of this link, which is the main subject of *Micromechanics* [1], is of relevant technological interest, as it may enable the design of materials with specific requirements by means of suitable manipulations of the microstructure.

Polycrystalline materials are used in many technological applications. Their microstructure is characterized by the grains morphology, size distribution, anisotropy, crystallographic orientation, stiffness and toughness mismatch and by the physical-chemical properties of the intergranular interfaces. These aspects have a direct influence on the initiation and evolution of micro-damage, which is also sensitive to the presence of micro-imperfections. Any theory trying to explain the failure mechanisms in these materials must then accommodate a relevant number of parameters.

In this study, a novel 3D *grain-boundary* micro-mechanical model for the analysis of intergranular degradation and failure in polycrystalline materials is presented. The microstructure is generated by means of *Voronoi tessellations*, able to retain the main statistical features of polycrystals. The formulation is built on a *boundary integral representation* of the elastic problem for the crystals, that are modeled as 3D anisotropic elastic domains with arbitrary orientation [2]. This representation involves only mechanical variables at the grains interfaces, i.e. displacement jumps and tractions, that play an important role in the micromechanics of polycrystals. The aggregate integrity is restored by enforcing suitable intergranular conditions. The onset and evolution of intergranular damage is modeled using an *extrinsic irreversible cohesive law*, able to address mixed-mode failure conditions. Upon interface failure, a *non-linear frictional contact analysis* is used, to address separation, sliding or sticking between the formed micro-crack surfaces. The incremental-iterative algorithm for tracking the micro-evolution is presented. Several numerical tests on pseudo and fully three-dimensional microstructures are discussed. The present formulation is a promising tool in the framework of *multiscale analysis of degradation and failure* in polycrystalline materials.

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References

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