Brittle failure in polycrystalline RVEs by a grain-scale cohesive boundary element formulation

I. Benedetti[1,2] and M.H. Aliabadi[1]

[1]Imperial College London, South Kensington Campus, SW7 2AZ, London, UK.
[2]Università degli Studi di Palermo, Viale delle Scienze, Edificio 8, 90128, Palermo, Italy.

e-mail: i.benedetti@imperial.ac.uk

Polycrystalline materials are commonly employed in engineering structures. For modern applications a deep understanding of materials degradation is of crucial relevance. It is nowadays widely recognized that the macroscopic material properties depend on the microstructure.
The polycrystalline microstructure is characterized by the features of the grains and by the physical and chemical properties of the intergranular interfaces, that have a direct influence on the evolution of the microstructural damage. The experimental investigation of failure mechanisms in 3D polycrystals still remains a challenging task.
A viable alternative, or complement, to the experiments is *Computational Micromechanics*. The present-day availability of cheaper computational power is favoring the advancement of the subject. A popular approach for polycrystalline fracture problems consists in the use of cohesive surfaces embedded in a Finite Element (FE) representation of the microstructure, so that the evolution of microcracks stems as an outcome of the simulation, without any assumptions, see e.g. [4].
An alternative to the FEM is the Boundary Element Method (BEM). A 2D cohesive BE formulation for intergranular failure and a 3D BE formulation for polycrystalline materials homogenization have been recently proposed [1–3].
In this work, a novel 3D grain-level model for the study of polycrystalline intergranular degradation and failure is presented. The microstructures are generated as Voronoi tessellations, that mimic the main statistics of polycrystals. The formulation is based on a grain-boundary integral representation of the elastic problem for the crystals, seen as anisotropic domains with random crystallographic orientation in space. The integrity of the aggregate is restored by enforcing suitable intergranular conditions. The evolution of intergranular damage is modeled using an extrinsic irreversible mixed-mode cohesive linear law. Upon interface failure, 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 micro-cracking evolution. Several numerical tests have been performed and they demonstrated the capability of the formulation to track 3D micro-cracking, under either tensile or compressive loads.

Acknowledgments This research was supported by a Marie Curie Intra-European Fellowship within the 7th European Community Framework Programme (Project No 274161).

References

[1] I. Benedetti and M. H. Aliabadi. A three-dimensional grain boundary formulation for microstructural modelling of polycrystalline materials. *Computational Materials Science*, 67:249–260, 2013.
[2] I. Benedetti and M. H. Aliabadi. A grain boundary formulation for the analysis of three-dimensional polycrystalline microstructures. *Key Engineering Materials*, 525-526(1):1–4, 2013.
[3] G. K. Sfantos and M. H. Aliabadi. A boundary cohesive grain element formulation for modelling intergranular microfracture in polycrystalline brittle materials. *International Journal for Numerical Methods in Engineering*, 69:1590–1626, 2007.
[4] I. Simonovski and L. Cizelj. Computational multiscale modeling of intergranular cracking. *Journal of Nuclear Materials*, 414(2):243 – 250, 2011.