

# Effects of voids and flaws on mechanical properties, and on intergranular damage and fracture for polycrystalline materials.

G. Geraci<sup>1,2</sup>, I. Benedetti<sup>1,2</sup> and M.H. Aliabadi<sup>3</sup>

<sup>1</sup>Dipartimento di Ingegneria Civile, Ambientale, Aerospaziale e dei materiali, Università degli Studi di Palermo, Viale delle Scienze, Edificio 8, 90128, Palermo, Italy

<sup>2</sup>Department of Aeronautics, Imperial College London, South Kensington Campus, SW7 2AZ, London, UK.

[giorgio.geraci13@imperial.ac.uk](mailto:giorgio.geraci13@imperial.ac.uk), [giorgioGeraci882@gmail.com](mailto:giorgioGeraci882@gmail.com), [i.benedetti@imperial.ac.uk](mailto:i.benedetti@imperial.ac.uk),  
[ivano.benedetti@unipa.it](mailto:ivano.benedetti@unipa.it), [m.h.aliabadi@imperial.ac.uk](mailto:m.h.aliabadi@imperial.ac.uk)

**Keywords:** Polycrystalline materials, Micromechanics, Material homogenization, Grain boundary, Cohesive zone model, Intergranular fracture, Porosity, Boundary element method

**Abstract.** It is widely recognized that the macroscopic material properties depend on the features of the microstructure. The understanding of the links between microscopic and macroscopic material properties, main topic of Micromechanics, is of relevant technological interest, as it may enable the deep understanding of the mechanisms governing materials degradation and failure. Polycrystalline materials are used in many engineering applications. Their microstructure is determined by distribution, size, morphology, anisotropy and orientation of the crystals. It worth noting that also the physical-chemical properties of the intergranular interfaces, as well as the presence of micro-imperfections within the microstructure, have to be taken into account, as they may have to a strong influence on onset and evolution of damage.

In this study, a two-dimensional micro-mechanical model for the determination of the effective or overall properties of polycrystalline materials, at the macroscopic scale, is presented. Furthermore, the evolution of intergranular degradation and failure is studied. The microstructures are generated by means of Voronoi tessellations, since they describe well the statistical features of polycrystalline materials. Each grain is assumed as a single crystal with general elastic orthotropic mechanical behaviour, and is discretized using the proposed anisotropic boundary element method, considering the random location, morphology and material orientation of each grain [1,2]. The variables used to describe the interface status are only the mechanical ones, i.e. tractions and displacement jumps. Crack onset and propagation along the grain boundaries interfaces are modelled using a linear cohesive law, considering mixed mode failure conditions. Upon interface failure, a non-linear frictional contact analysis is used to deal with separation, sliding or sticking between the cracked interfaces. The effect of randomly located pre-existing flaws on the overall behaviour and micro-cracking evolution of a polycrystalline material is also investigated, as well as the effect of missing grains within the structure, modelling in this way the presence of voids among crystals (porosity).

## References

- [1] G. K. Sfantos, 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 (2007) 1590–1626.
- [2] I. Benedetti, M.H. Aliabadi, A three-dimensional grain boundary formulation for microstructural modelling of polycrystalline materials, *Computational Materials Science*, 67, 249-260, 2013.