A multiscale and multi-physics boundary integral model for polycrystalline materials including damage initiation and evolution under different loading scenarios

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Polycrystalline materials, either metals, ceramics or alloys are ubiquitous all sectors of engineering. The macroscopic properties of polycrystalline components, including the initiation and evolution of damage and its transition from the microstructural level – the *material* scale – to the macrostructural level – the *component* scale – depend on the morphological and constitutive features of the crystals and their intergranular interfaces.

Thanks to the remarkable momentum gained by experimental materials nano/micro-characterisation on one side and high performance computing (HPC) on the other side, the last few decades have witnessed the tremendous development of the paradigms of *multi-scale materials modelling* and *materials by design* [1], where the emerged experimental and computational capabilities are combined in the attempt to understand and explain complex hierarchical material behaviours first and to employ the gained knowledge to design novel materials, through the fine control of their micro-structure, then.

Despite the wider affordability of HPC, fully 3D multiscale computations remain a daunting task, especially when highly non-linear phenomena, such as initiation and evolution of damage, phase changes, etc. are considered. For such a reason, the development of computationally effective, accurate and reliable formulations remain an important task, which complements progress in computing hardware as well as in costly experimental equipment.

In this context, the present contribution reviews the recent development of a computational framework for multiscale analysis of polycrystalline components subject to different loading scenarios and including the evolution of material damage and cracking [2, 3]. The underlying formulation employs generalised Voronoi tessellations for representing the material micro-morphology and boundary integral equations for modelling of the fully anisotropic behaviour of the constituent grains. The initiation and evolution of either inter- or trans-granular damage and cracking is represented through cohesive traction-separation relationships that, by virtue of their mathematical form, are conveniently coupled with the integral equations modelling the behaviour of the individual crystals.

The use of the developed framework for computational homogenization a micro-cracking analysis of polycrystalline aggregates under either monotonic quasi-static loading, low or high cycle fatigue, in presence of hydrogen embrittlement or thermo-mechanical loads is illustrated [4]. It is also shown how the tool can be used for investigating the inter/trans-granular cracking competition and for analysing piezoelectric aggregates. Eventually, the development of a BE^2 framework is described and possible future developments of the presented formulation are discussed.

References

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