Multi-scale and multi-physics modelling of polycrystalline materials by the boundary element method

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Abstract

Polycrystalline materials are widely employed for engineering applications in several sectors, ranging from the civil to the aerospace and biomedical fields. Their macroscopic behavior depends on the morphological and constitutive features of the crystals comprising their microstructure and on the complex mechanisms localized at the intergranular interfaces. Recent developments in microscopy, on the one hand, and in high-performance computing, on the other hand, have allowed the development of complex computational tools able to capture complex non-linear behaviors of such materials, including the nucleation of damage at the micro-scale and its transition to the component level, where it can affect the functionality and, in some cases, the safety of the considered engineering system.
In this context, the present contribution describes the development of a novel computational framework based on boundary elements for the multiscale and multi-physics analysis of polycrystalline materials, capable of representing the initiation, coalescence, evolution of micro-damage and cracking. The formulation underpinning the computational tool is based on the employment of *generalized Voronoi tessellations* as a representation of the material micro-morphology and of *boundary integral equations* for modelling of the fully anisotropic behavior of the individual crystals. The localization of inter-/trans-granular damage and cracking is modelled through *cohesive traction-separation relationships*, which are conveniently coupled with the integral equations modelling the crystals mechanics.

The developed framework has been successfully employed for computational homogenization and micro-cracking analysis of polycrystalline specimens subject to either quasi-static monotonic loading, low or high cycle fatigue, and in presence of hydrogen embrittlement or thermo-mechanical loads. It has also been used for investigating the inter/trans-granular cracking competition and for analyzing piezoelectric aggregates. Eventually, the development of a two-scale methodology is described and potential future developments are discussed.

References

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