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A 3D multi-physics boundary element computational framework for polycrystalline materials micro-mechanics

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Abstract: A recently developed novel three-dimensional (3D) computational framework for the analysis of polycrystalline materials at the grain scale is described in this lecture. The framework is based on the employment of: *i*) 3D *Laguerre-Voronoi tessellations* for the representation of the micro-morphology of polycrystalline materials; *ii*) *boundary integral equations* for the representation of the mechanics of the individual grains; *iii*) suitable *cohesive traction-separation laws* for the representation of the multi-physics behavior of the interfaces (either inter-granular or trans-granular) within the aggregate, which are the seat of damage initiation and evolution processes, up to complete de-cohesion and failure. The lecture will describe the main features of the proposed framework, its main advantages, current issues and direction of potential further development. Several applications to the computational analysis of damage initiation and micro-cracking of common and piezoelectric aggregates under different loading conditions will be discussed. The framework could find profitable application in the multiscale analysis of polycrystalline components and in the design of micro-electromechanical devices (MEMS).

Keywords: Polycrystalline materials; Computational micro-mechanics; Multiscale materials modeling; Boundary element method

Background and outline

Polycrystalline materials, either metals, alloys or ceramics, are extensively used in engineering applications and they have long been investigated by materials scientists and engineers, with the aim of understanding and explaining their features and making their employment effective, safe and reliable.

In the last few decades, thanks to remarkable advancements in *microscopic materials characterization*, see e.g. Ref. [1], the interest of investigators has slowly shifted from a *phenomenological* description towards a *physically based* explanation of materials features, based on and fed by the enhanced available microstructural information. Concurrently, the rapid advancements in *high performance computing* have allowed the computational mechanics community to develop richer and more refined materials models, accommodating the wealth of available information provided by the emerging experimental methodologies. In this background, the novel paradigm of *multiscale material modeling* has emerged as a consistent framework attempting, often successfully, to link the microstructural description to the macroscopic properties of materials [2, 3].

In this background, the present lecture will describe a novel, recently developed, three-dimensional (3D) computational framework for the analysis of polycrystalline materials at the grain scale. The framework is based on the employment of: *i*) 3D *Laguerre-Voronoi tessellations* for the representation of the micro-morphology of polycrystalline materials; *ii*) *boundary integral equations* for the representation of the mechanics of the individual grains; *iii*) suitable *cohesive traction-separation laws* for the representation of the multi-physics behavior of the interfaces (either inter-granular or trans-granular) within the aggregate, which are the seat of damage initiation and evolution processes, up to complete de-

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cohesion and failure.

Differently from other popular approaches, the use of boundary integral equations offers some definite modeling advantages: *a*) they allow to express the overall problem in terms of interface variables only, namely displacement jumps and tractions, which are the variables directly entering the damage initiation and evolution processes; *b*) their form allows straightforward coupling with the cohesive equations, formulated directly in terms of tractions as a function of interface displacement jumps; *c*) their *boundary* nature requiring only the discretization of the surface of the individual crystals, they offer some simplification in analysis data preparation and a reduction of the overall number of degrees of freedom for the aggregate analysis (these advantages are partly maintained even in the case of non-liner constitutive behavior of the grains, including crystal plasticity).

The lecture will show how a general aggregate equation format, coupled with specific hybrid cohesive laws and suitable evolution rules, embodying an irreversible damage parameter, can be used for several applications including: *a*) computational homogenization of common and piezoelectric aggregates [4-6]; *b*) inter- and trans-granular damage and micro-cracking under quasi-static loading [6-9]; *c*) environmentally assisted micro-cracking and hydrogen embrittlement [10]; *d*) high-cycle fatigue micro-cracking [11]; *e*) micro-cracking of piezoelectric aggregates [5]; *f*) crystal plasticity [12]; *g*) multiscale analysis of polycrystalline components [13].

The key aspects [14] and general advantages of the methodology as well as some current issues or limitations will be discussed, together with possible further development directions. The lecture will show how the developed framework could be a valuable tool for multiscale analysis of polycrystalline components and for the design of micro-electro-mechanical devices (MEMS).

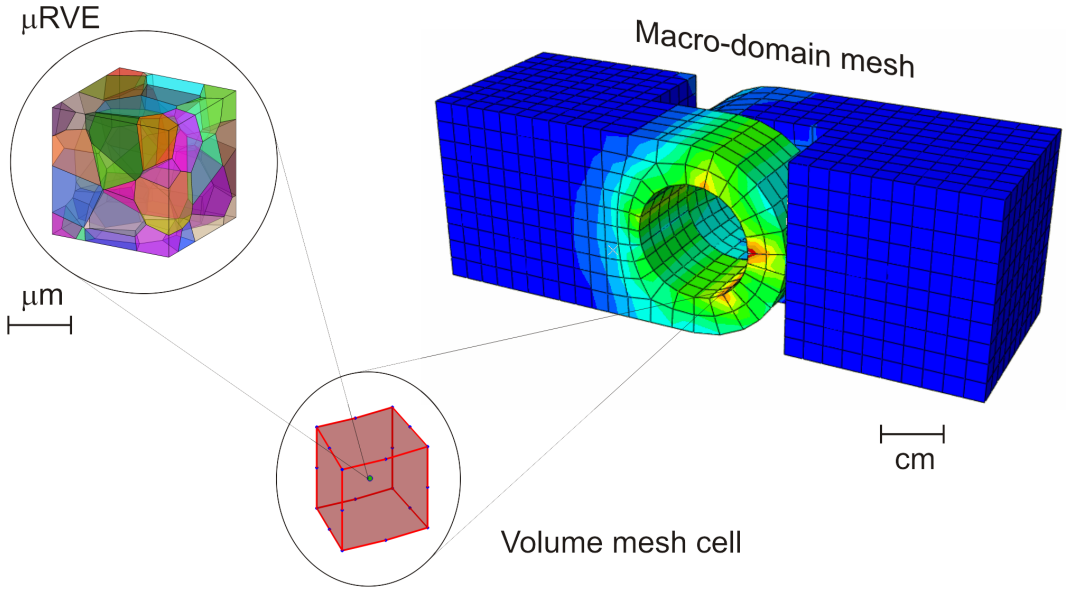

Fig.1: A schematic illustration of multiscale modeling of polycrystalline components.

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