SEMINAR

Micromechanical Modeling of Crystalline Interfaces

Aurélien Vattré
DMAS, ONERA, Université Paris-Saclay

Abstract

Interfaces, whether grain boundaries in polycrystalline materials or heterointerfaces in multiphase solids, are ubiquitous in materials science and engineering. Far from being simple separation surfaces between neighboring crystals, understanding the role of solid-solid interfaces represents a major challenge, requiring advanced theoretical and numerical strategies to describe their physical and mechanical characteristics.
The first part of this presentation is dedicated to microstructures dominated by interfaces, resulting from polymorphic (diffusionless) phase transformations. Under high hydrostatic compression and shock wave conditions, pressure-induced phase transitions and the formation of diffuse internal interfaces in iron are modeled within a thermodynamically coherent framework, combining nonlinear elastoplasticity and a multivariate phase-field approach adapted to large deformations.
The second part focuses on the detailed description of imperfect interfaces, particularly semi-coherent interfaces, characterized by networks of geometrically necessary dislocations that induce a deformation preserving lattice invariance. This deformation disrupts the uniformity of crystallographic correspondence across the interface, thereby reducing coherence. A constitutive law, integrating the contribution of geometrically necessary dislocations and designed for high-performance calculations on complex structures (in particular turbine blades), will also be presented.

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