

Multiscale modeling of polycrystalline materials

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This symposium aims to bridge the gap between microstructural phenomena and macroscopic properties of polycrystalline materials (either metals, alloys or ceramics) by exploring advanced modeling techniques across multiple scales. The study of polycrystalline materials is fundamental in numerous academic programs as well as in several industrial applications. The symposium will delve into the latest computational approaches to understand and predict the behavior of polycrystalline materials under various thermomechanical conditions.

Key topics will include:

- **Fundamental mechanisms:** Exploration of grain boundary dynamics, phase transformations, and mechanical properties at the atomic, micro and macro scales.
- **Modeling techniques for defects description:** Discussion on the integration of continuum mechanics, discrete dislocation dynamics, and crystal plasticity finite element methods. Complexion and disconnection-based approaches/models will be highly appreciated.
- **Numerical methods dedicated to mesoscopic description of grain and phase boundaries:** Vertex, Monte-Carlo, Cellular- Automaton, Multiphase field and level-set methods.
- **Innovative computational tools:** development of cutting-edge software and algorithms that enhance the scalability and accuracy of multiscale models, including virtual and boundary element methods.
- **Multiscale methods** for tracking the initiation of damage at the micro/meso-scale and its transition to the macroscale.
- **Application-Specific Models:** Focus on the customization of applicative models in the industry where polycrystalline structures are pivotal.
- **Machine learning strategies** for polycrystalline micro-mechanics, homogenization, grain boundary migration, phase transformation, damage and fracture mechanics.