Computational Crystal Plasticity for the Design of Materials and Processes

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ABSTRACT

The macroscale mechanical behaviour of crystalline materials, such as polycrystalline metals and single crystal semiconductors, is dictated by the anisotropic behaviour of individual crystals/grains and their interactions with neighboring crystals or other materials. Furthermore, the elastic-plastic response of individual crystals is associated with the underlying atomic lattice structure and phenomena of dislocation glide on the slip systems and dislocation multiplication and interactions. As a result, microstructural characteristics such as grain size, shape, and orientation, have a significant effect on the macroscale mechanical properties and performance. Moreover, these microstructural features are strongly affected by the thermal-mechanical process used to create a part. Because of this, tremendous effort has been made to develop crystal plasticity models that explicitly model the crystal (grain) scale behavior to predict the local macroscale response.

In this talk, a framework for computational modelling of discretized single or polycrystal grain structures subjected to thermal-mechanical loading conditions is presented. The model is general for finite deformations with the crystal plasticity model based on dislocation motion and interactions. A parallel finite element implementation is briefly described. Then, applications including predicting microstructure evolution during large deformation processing, fatigue crack initiation, and defect formation during single crystal AlN crystal growth will be presented.

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