THE DEPARTMENT OF CIVIL ENGINEERING

ANNOUNCES THE THESIS DEFENSE OF

Doctoral Candidate

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"Crystal Plasticity FE Models for Predicting Deformation and Twinning in Polycrystalline Magnesium Alloys"

Abstract

Magnesium alloys exhibit complex deformation related mechanical behavior, viz. plastic anisotropy, tension-compression asymmetry and premature failure. Their origins are in the underlying heterogeneous deformation due to dislocation slip and deformation twinning on different crystallographic systems. The twin formations lead to microstructure evolution, strain localization and initiation of short cracks. Reliable prediction of mechanical response and failure is predicated upon the ability of computational models of polycrystalline microstructures to accurately simulate the heterogeneous twin-formation and deformational localization.

In this dissertation, a modeling framework is developed for crystal plasticity finite element (CPFE) simulation of deformation and explicit micro-twin formation in the image-based virtual polycrystalline microstructures of Mg alloys. The model accounts for dislocation slips, geometrically necessary dislocations (GNDs) accumulations, stress concentration near grain boundaries and the explicit micro-twin nucleation-propagation. The micro-twin nucleation is modeled based on energy-partitioning following the dislocation dissociation process. The micro-twin propagation and associated localized plastic flow are described with novel crystal plasticity constitutive relations derived from micro-mechanisms. The models predict the twin-evolution-induced material responses at multi-scales, including at macroscopic scale the tension-compression asymmetry and the dramatic change of hardening rates due to twin activity, as well as at microscopic scale the dislocation density distribution and stress concentration in the twined microstructures which are potentially responsible for short-crack initiation.

Two difficulties rise from the numerical implementation of the proposed CPFE twin models. Firstly the linear shape function four-node tetrahedral (TET4) elements which are used to represent the tortuous geometry of the grains exhibit significant volumetric locking in the plastic deformation regime and thus predict inaccurate CPFE results. Especially, significantly premature micro-twin nucleation time is predicted by linear TET4 elements. To stabilize the CPFE twin simulation, a locally integrated B-bar (LIB) element and a F-bar patch (FP) based element are developed using selectively reduced iteration of the constitutive relations within a node-based and a tetrahedron-based patch, respectively. The new elements are validated through comprehensive simulation tests in single crystal, bi-crystal and poly-crystals with various loadings.

The other problem comes from the fact that the micro-twin formation intensifies the simulation time steps with deformation localization within twin bands. High resolution meshes required to discretize the tortuous grain geometry combined with very fine time steps increases the computation cost enormously and makes high-fidelity CPFE simulation of polycrystalline Mg alloys infeasible. A subcycling temporal integration algorithm for multi-time-scale CPFE twin simulation is developed to improve the simulation efficiency. The algorithm separates the FE domain into sub-domains with different critical time steps. Each sub-domain updates the stress and the deformation-dependent variables in different rates, followed by a coupling to satisfy the global equilibrium at the end of every coarsest time step. Using the subcycling algorithm, significant acceleration is observed in CPFE twin simulations without compromising on the accuracy. The CPFE twin models, stabilized and accelerated with the proposed numerical methods, predict the microstructure-property relations and set the stage for studying the failure initiation in single and polycrystalline Mg alloys.

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