# THE DEPARTMENT OF CIVIL ENGINEERING

ANNOUNCES THE THESIS DEFENSE OF
Doctoral Candidate

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Tuesday, August 25, 2015
3:00-5:00pm
Latrobe 106

## "Distribution Enhanced Methods of Homogenization for Heterogeneous Materials and Multi-scale Crystal Plasticity Modeling"


Abstract

Ductile rupture is the dominant failure mechanism in body centered cubic (BCC) tantalum (Ta) loaded at high strain rates. Existing material models and simulation techniques are insufficient to provide the desired level of fidelity and accuracy in representing the plasticity and damage evolution in this dynamic failure process. Significant advancement is required to model the effects of the contributing physical processes, which play out over a range of length and timescales covering multiple orders of magnitude, and to incorporate these effects into a single coherent simulation framework.

In this study, the authors propose a novel multiscale framework for modeling ductile failure with crystal plasticity and damage. Within this framework, the single crystal plasticity constitutive behavior is derived from the results of molecular dynamics simulations, where the atomistic process of slip is modeled explicitly. These results are used to establish a physically meaningful functional form and parameterization for a continuum-scale crystal plasticity flow rule that captures the effects of loading orientation, strain rate, and temperature.

At the intermediate scale, slip and hardening and the coupling of these phenomena to the evolution of damage in the material are studied. Finite element simulations of damage evolution are performed with the atomistically-informed flow model coupled to dislocation density based crystal plasticity. Rates of slip and hardening are directly linked to dislocation kinetics and dislocation density evolution and structure formation at this scale. The spatial discretization at this scale includes an explicit geometric representation of damage as an initially spherical void that evolves during deformation. The effects of damage on the evolving plasticity are quantified, and an understanding of the role of crystal plasticity and stress triaxiality on damage evolution is obtained.

At the highest scale, finite element simulations employ a homogenized constitutive law that couples crystal plasticity and damage evolution. The heterogeneous stress field induced by the damage is handled within the newly developed distribution enhanced homogenization framework, where evolving measures of microscale stress distributions are explicitly included as new internal variables in the homogenized constitutive relation. This model accurately represents the material behavior observed at the intermediate continuum scale without explicit geometric representation of the damage. A novel damage evolution law is introduced to model void growth, and this model accurately represents the effects of the microscale stress field on the plastic evolution of the void and the surrounding material.


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