

HOMOGENIZATION-BASED MULTISCALE MODELING OF CRYSTAL PLASTICITY AND DUCTILE FAILURE AT HIGH STRAIN RATES

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Ductile rupture is the dominant failure mechanism in body centered cubic tantalum 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 via finite element simulations. At the lower, atomistic scale, the process of slip is modeled through molecular dynamics simulations to establish a physically meaningful functional form and parametrization for a crystal plasticity flow rule. The atomistic results quantify the effects of loading orientation, strain rate, and temperature that are necessary to include in the flow model.

At the intermediate scale, the evolution of slip and hardening and the coupling of these phenomena to the evolution of damage in the material are studied. Unit cell finite element simulations of damage evolution are performed using a constitutive model that implements dislocation density based crystal plasticity. Slip and hardening are directly linked to dislocation kinetics and dislocation density evolution and structure formation at this scale. The effects of damage on the evolving plasticity are quantified, and a model for damage evolution is extracted from the simulation results.

At the higher scale, finite element simulations are performed to model ductile failure in a heterogeneous polycrystalline medium. At this scale, homogenization-based constitutive models are employed to model the effects of damage and crystal plasticity. The simulations are used to study damage evolution and its eventual culmination in material failure.

In this presentation, the authors present results from unit cell calculations representing the intermediate scale that provide insight into the evolution of damage in an anisotropic single crystal and the plasticity that accompanies this process.

REFERENCES

- [1] C. Alleman, S. Ghosh, D. J. Luscher, and C. Bronkhorst, Evaluating the Effects of Loading Parameters on Single Crystal Slip in Tantalum Using Molecular Mechanics, *Phil. Mag.*, Vol. **94**, 92–116, 2014.