MULTICALE CRYSTAL PLASTICITY MODELING FOR METALS UNDER EXTREME CONDITIONS

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Focus Material: Metals

Focus of the Presentation: Physics-based multi-scale model development

Abstract

Crystal plasticity modeling is useful for considering the influence of anisotropy of elastic and plastic deformation on local and global responses in crystals and polycrystals. Modern crystal plasticity has numerous manifestations, including bottom-up models based on adaptive quasi-continuum and concurrent atomistic-continuum methods in addition to discrete dislocation dynamics and continuum crystal plasticity. Some key gaps in mesoscale crystal plasticity models will be discussed, including interface slip transfer, grain subdivision in large deformation, evolution of defects and deformation in irradiated materials, shock wave propagation in heterogeneous polycrystals, and dislocation dynamics with explicit treatment of waves. Given the mesoscopic character of these phenomena, contrasts are drawn between bottom-up (simulations and experimental observations) and top-down (experimental) information in assembling mesoscale constitutive relations and informing their parameters. Owing to the high utility of metastable structures in practice, kinetic pathways for mesoscale defect structures are considered. We consider requirements for coarse-graining of microstructure evolution across scales based on the notion of spatio-temporal activation volume averaging exploiting transition state theory.