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"Developing A Crack Propagation Model in the Metallic Materials from A Self-Consistent Coupled Atomistic-Continuum Model"

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Understanding failure process in metallic materials are crucial to their engineering applications. The complexity of failure analysis origins from the intrinsic nature that material failure couples various mechanisms across multiple spatial and temporal scales. The interaction between crack propagation and evolution of deformation mechanisms including dislocation and micro-twinning have strong impact on the failure process. While crack propagation models at macroscopic level such as cohesive zone model have made substantial progress in crack propagation studies, these models performs poorly at micron and sub-micron scale. One major reason is the lacking of representation of microstructure dependence and interaction between cracks and plastic deformations. There is considerable need to develop more physical based crack propagation model addressing the evolution of deformation mechanisms and their impact on crack propagation.

In this dissertation, a novel computational framework is developed to explicitly model the process of crack propagation and associated deformation mechanisms evolution with atomistic resolution. The development starts with building a robust on-the-fly tool to characterize and quantify the evolution of deformation mechanisms at the atomistic scale. To overcome the length scale limitation of molecular dynamics, a self-consistent atomistic and continuum coupling model is introduced using continuum model in the far field and atomistic model near crack tip. The coupling is achieved by enforcing geometric compatibility and force equilibrium condition in a weak sense at the interface region between two domains. The coupled model takes care of numerical error sources such as ghost-force and phonon-reflection and allows finite temperature applied in the atomistic domain in order to study the thermally activated processes. A nonlinear and nonlocal constitutive relation is used for the continuum domain to be consistent with inter-atomic potentials. The coupled model is solved iteratively using LAMMPS as simulator of atomistic system and finite element code for continuum system, both efficiently implemented in parallel and communicating using MPI library.

The orientation dependence of nucleation and evolution crack tip deformation mechanisms and its correlation between mechanical behavior is revealed by characterization tool in atomistic simulation. Crack tip field and propagation process is studied using the coupled concurrent model. The simulation shows a transition between crack propagation and dislocation nucleation as dominated mechanism for different orientations which is analyzed using Peierls model. The crack propagation is found to follow specific low index plane, a rate form of crack propagation law is extracted from the simulation results. In the dislocation dominated scenario, a dislocation density based information passing model is introduced to incorporate the plastic deformation into the coupled model validated by correlating distribution of dislocation density with plastic deformation rate in the interface region.