# Linking Mesoscale Plasticity to Atomistics

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## ABSTRACT

Dislocation interactions and failure mechanisms at mesoscopic length scales of metallic materials are usually out of reach of atomistic simulations, thus requiring effective continuum models to describe their collective behavior and the resulting constitutive response. Coarse-graining the crystalline atomic ensemble, e.g. by means of the quasicontinuum (QC) approximation [1,2] combined with techniques to accelerate atomistic simulations [3], provides an avenue to locally retain atomistic accuracy while being applicable to larger scales. One such method, the fully-nonlocal energy-based QC technique [4,5] allows us to simulate the response of crystalline solids solely based on interatomic potentials but at significantly larger length scales than conventional molecular dynamics (MD). Here, we will apply this approach to study defect mechanisms in representative copper and aluminum single- and polycrystals. Among others, we will demonstrate the importance of coarse-grained atomistic simulations to avoid modeling artifacts inherited from nanoscale MD simulations.

Void nucleation, growth and coalescence are important mechanisms responsible for spall and ductile failure. By simulating individual nano-voids and collections of voids under hydrostatic and multiaxial loading, we investigate (i) the nucleation of defects and the associated failure mechanisms at sufficiently-large loads, and (ii) the importance of coarse-grained atomistic techniques to avoid modeling artefacts and size effects in small representative volume elements treated by conventional atomistic methods.

Grain boundaries (GBs) play a central role in polycrystal plasticity through their interactions with lattice defects as well as through GB relaxation mechanisms. We will use the aforementioned coarse-grained atomistic technique to study the behavior of GBs in three-dimensional crystals with a particular focus on the GB strength and the interaction with dislocations. As in the case of void expansion, the QC simulations enable us to consider sample sizes outside the realm of conventional atomistic techniques.

## REFERENCES

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