PREDICTING METAL PLASTICITY THROUGH CROSS-SCALE MODELING

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Metal plasticity lies at the heart of many engineering applications, yet exactly how metals deform under load and how the resulting microstructure affects material properties is still not fully understood. In this talk, I will review our recent progress on how direct molecular dynamics (MD) simulations of crystal plasticity with up to billions of atoms provide an unprecedented opportunity to elucidate the fundamental mechanisms of plasticity with atomic resolution, giving us access to information that is difficult or impossible to obtain through experiments. I will exemplify our cross-scale approach on the cases of single crystals, bi-crystals, and alchemical models to study complex alloys. Altogether, this approach provides a new framework for fundamental understanding and for developing high-fidelity models of metal behavior from the atomistic to the mesoscopic and macroscopic scales.

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