UMENO LAB.

Challenges to Nano-Micro Mechanophysics and Multiscale Simulation

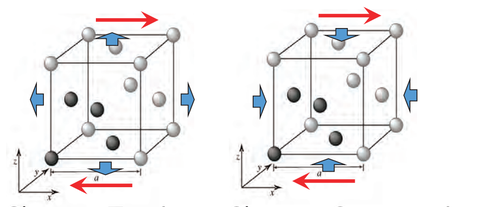
Department of Fundamental Engineering
Center for Research on Innovative Simulation Software

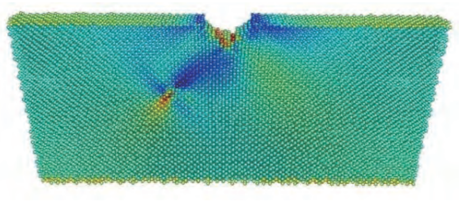
Nano-Micro Mechanophysics
Department of Mechanical Engineering, Graduate School of Engineering
https://www.cmsm.iis.u-tokyo.ac.jp/en/

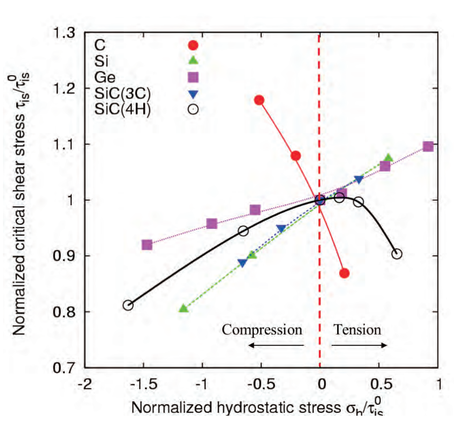
Unveiling Nano-Micro Mechanophysics for hierarchical Multiscale Simulation

We aim to reveal the mechanical and physical properties of nanomaterials by ab initio density functional theory calculations and molecular dynamics simulations. We also work on multiscale simulation based on knowledge of nano-microscale phenomena.

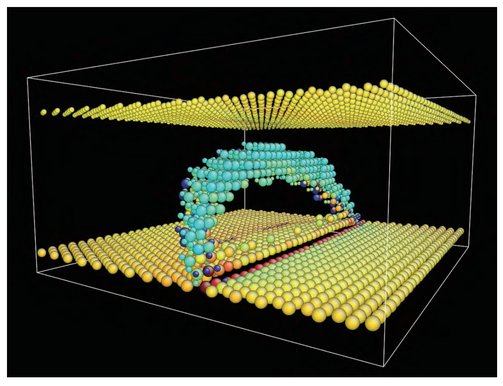
Atomistic simulation of crystal strength





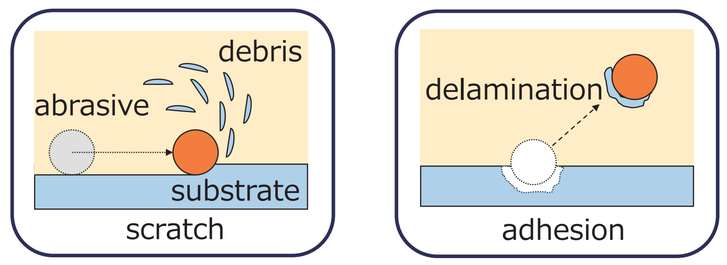


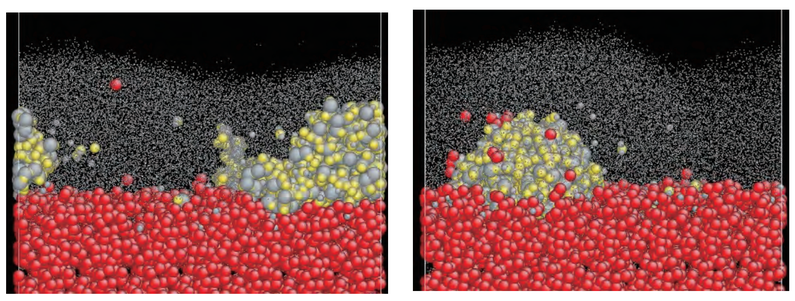
Ideal shear stress (ISS) under compression/tension in covalent crystals



Molecular dynamics simulations of dislocation motion and crystal slip

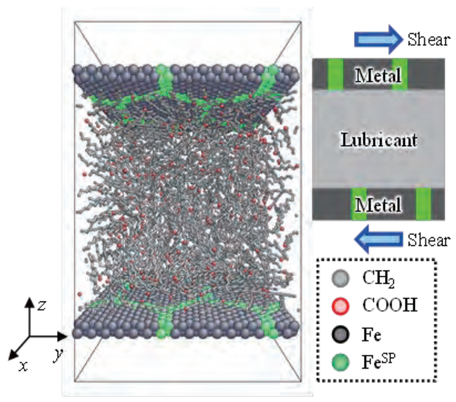
Reactive molecular dynamics simulation of CMP

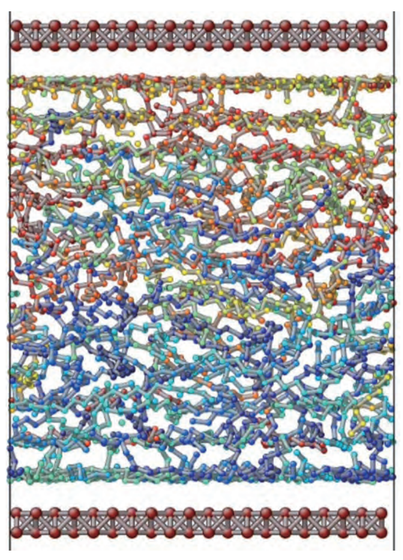


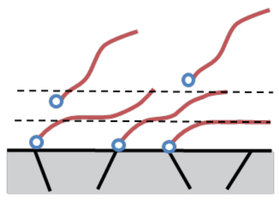


Atomistic model simulation of material removal mechanisms by scratch ad adhesion in CMP (chemical mechanical planarization)

Molecular simulation of boundary lubrication

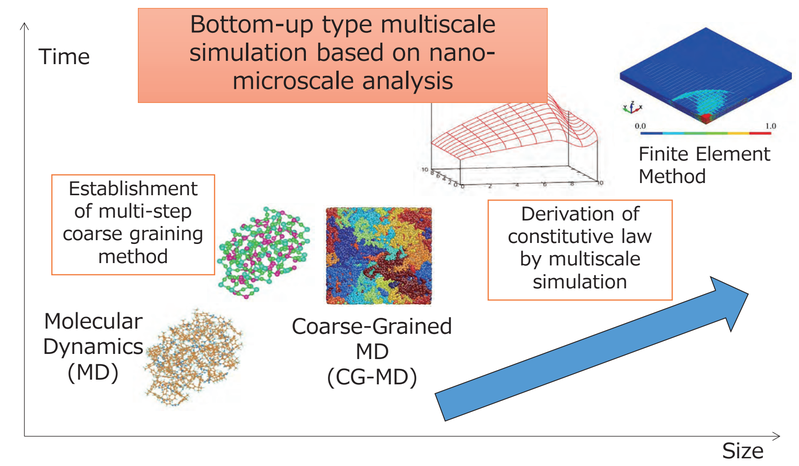


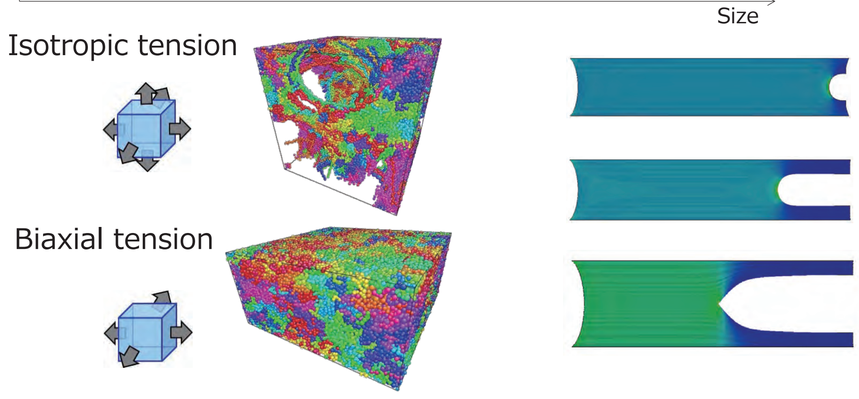




Coarse-grained molecular dynamics simulation of formation of lubricant molecule structure (polymer brush) on metal surface with nanograins

Multiscale simulation of polymer materials





Coarse-grained MD simulation

FEM analysis of crack propagation