CISS

UMENO LAB.

[Modeling and Simulation of Nano-Micro Mechanophysics]

Center for Research on Innovative Simulation Software

Nano-Micro Mechanophysics

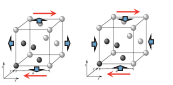
Dept. of Mechanical Engineering

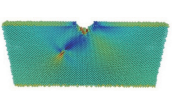
http://www.cmsm.iis.u-tokyo.ac.jp

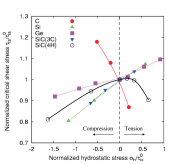
Challenges to Nano-Micro Mechanophysics and Multiscale Simulation

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.

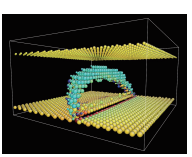
Atomistic simulation of crystal deformation and fracture





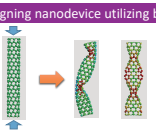


Ideal shear stress (ISS) under compression/tension in covalent crystals

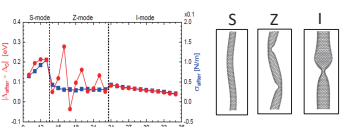


Molecular dynamics simulations of dislocation motion and crystal slip

Designing nanodevice utilizing buckling deformation

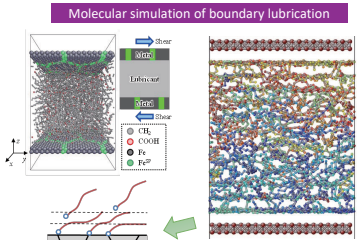


Atomistic model analysis of buckling behavior of carbon nanotubes under axial compression



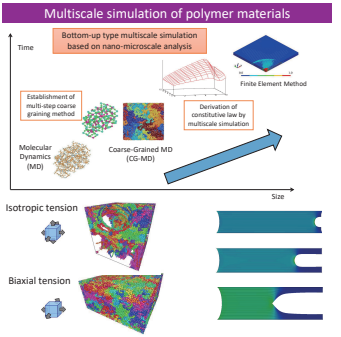
Nanotube diameter vs. buckling mode, buckling-induced band gap change, and post-buckling stress

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