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
- Designing nanodevice utilizing buckling deformation
- Multiscale simulation of polymer materials

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

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

Coarse-grained MD simulation

Multiscale simulation of polymer materials

Establishment of multi-step coarse-graining method

Molecular dynamics (MD)

Coarse-grained MD (CG-MD)

Isotropic tension

Biaxial tension

Coarse-grained MD simulation

FEM analysis of crack propagation