

UMENO LAB.

Unveiling Nano-Micro Mechanophysics for hierarchical Multiscale Simulation



Department of Fundamental Engineering
Center for Research on Innovative Simulation Software

Nano-Micro Mechanophysics

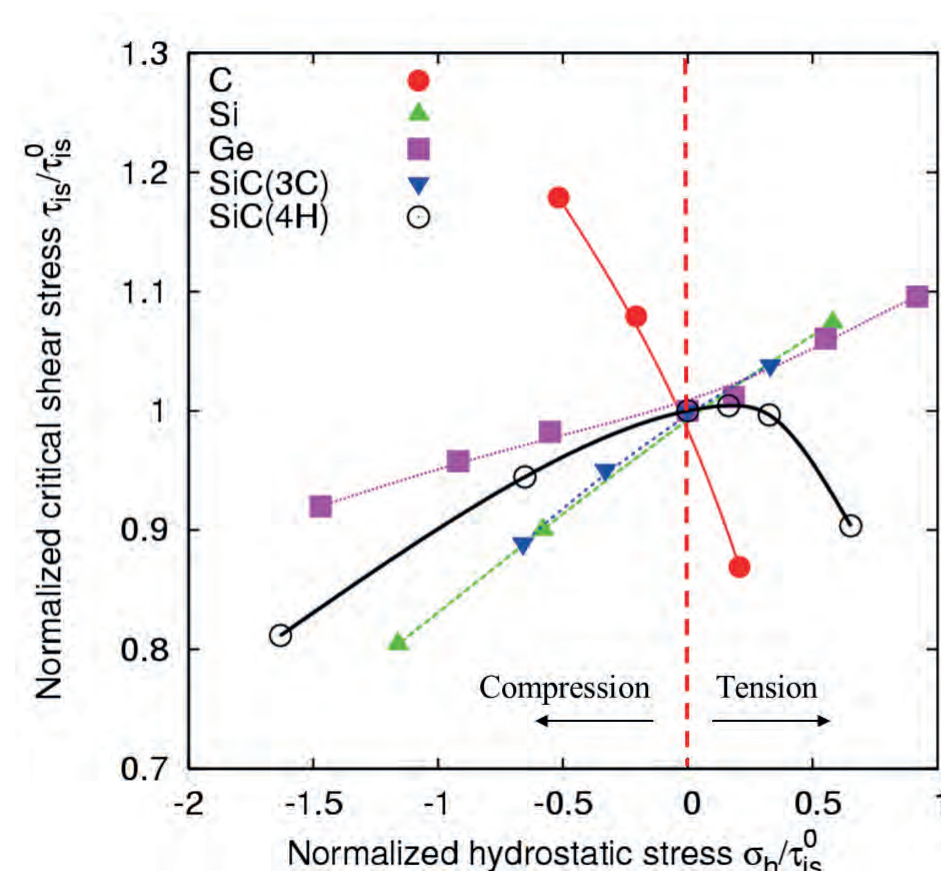
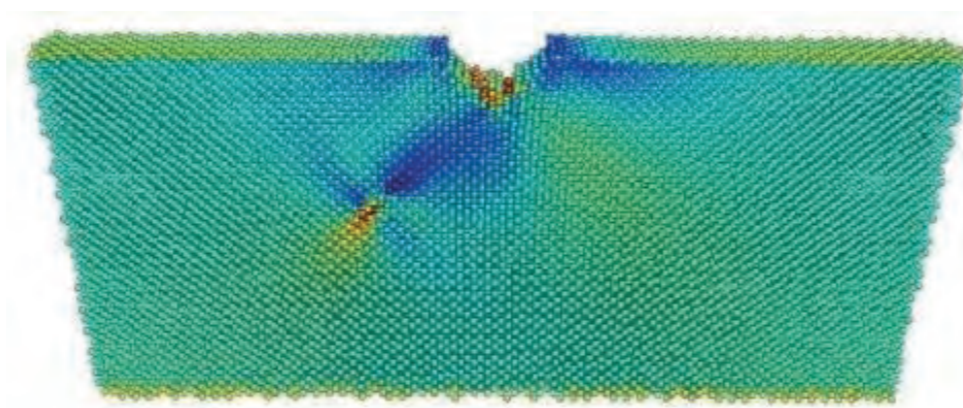
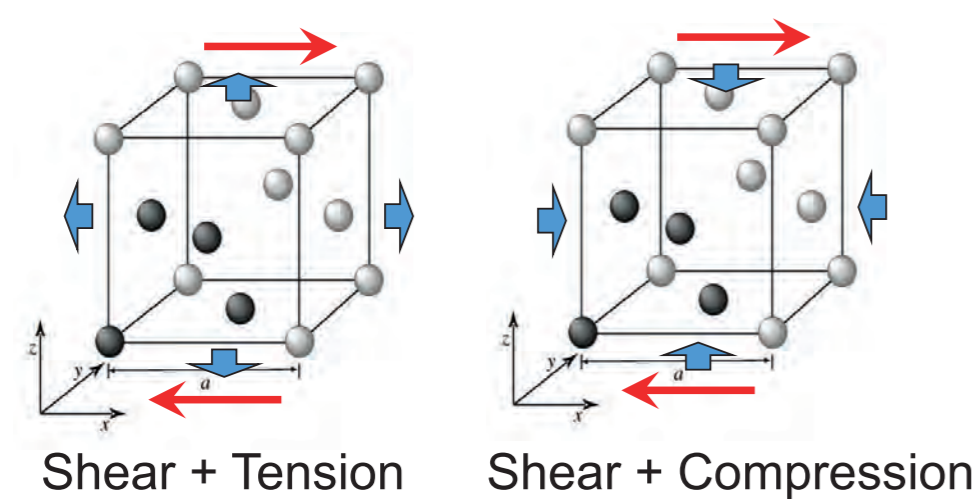
Department of Mechanical Engineering, Graduate School of Engineering

<http://www.cmsm.iis.u-tokyo.ac.jp/en/index.html>

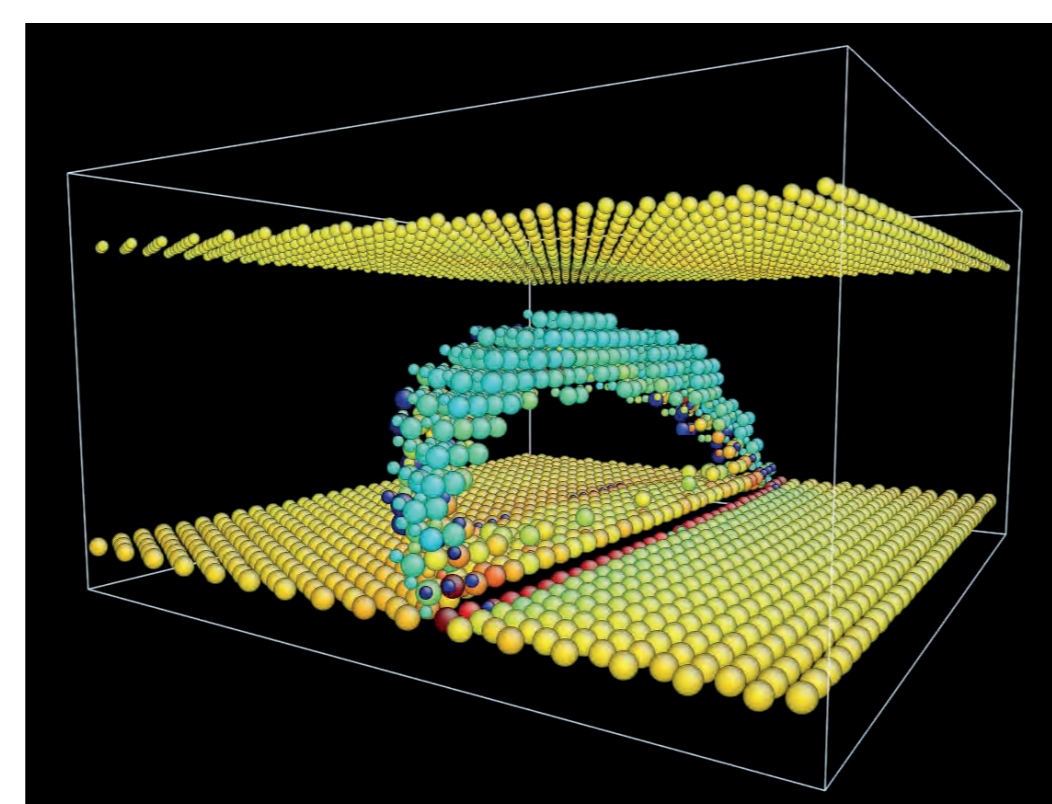
Unveiling Nano-Micro Mechanophysics for hierarchical Multiscale Simulation

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 deformation and fracture

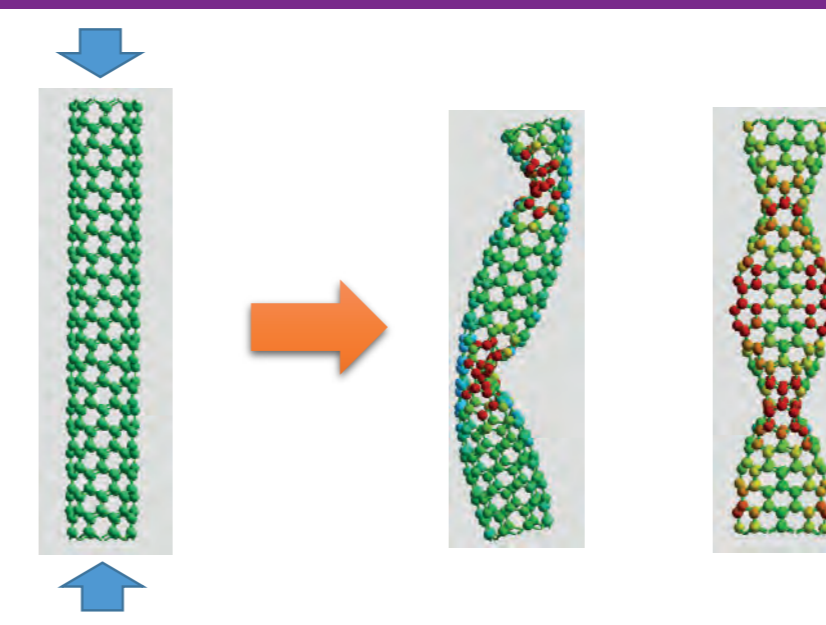


Ideal shear stress (ISS) under compression/tension in covalent crystals

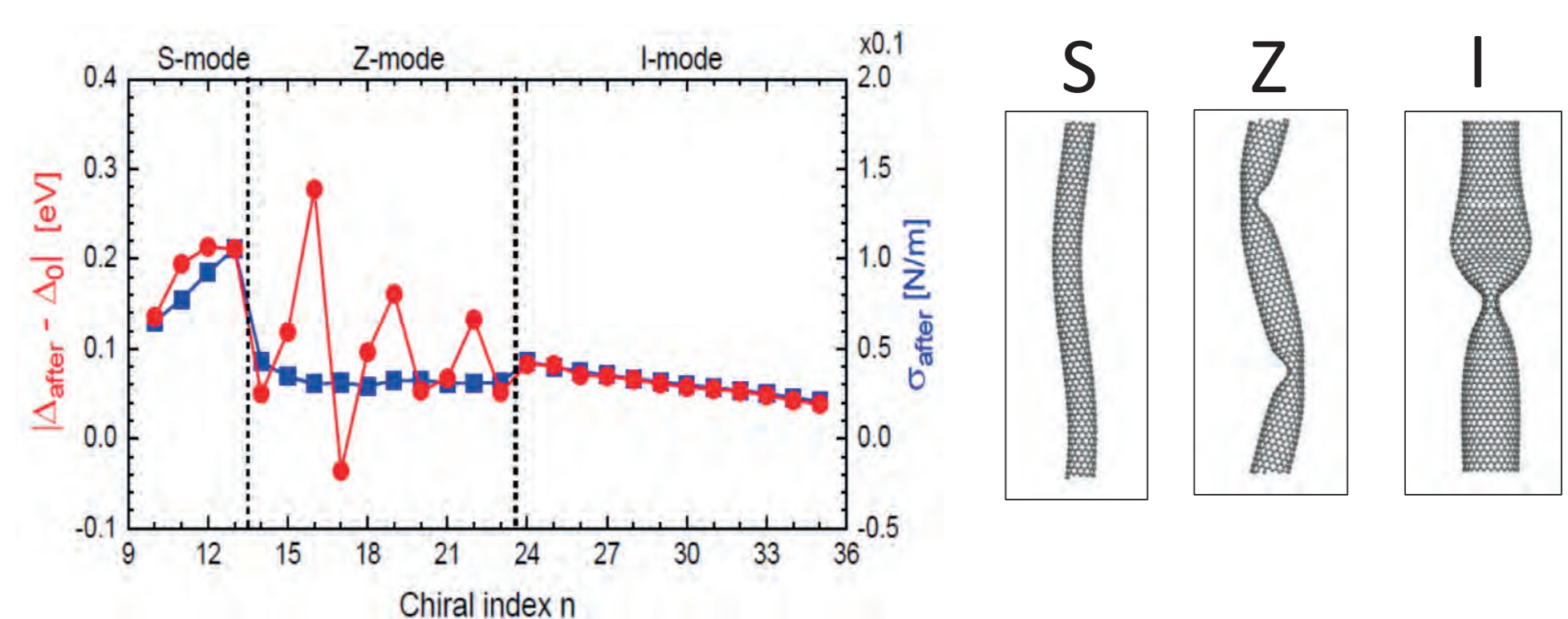


Molecular dynamics simulations of dislocation motion and crystal slip

Designing nanodevice utilizing buckling deformation

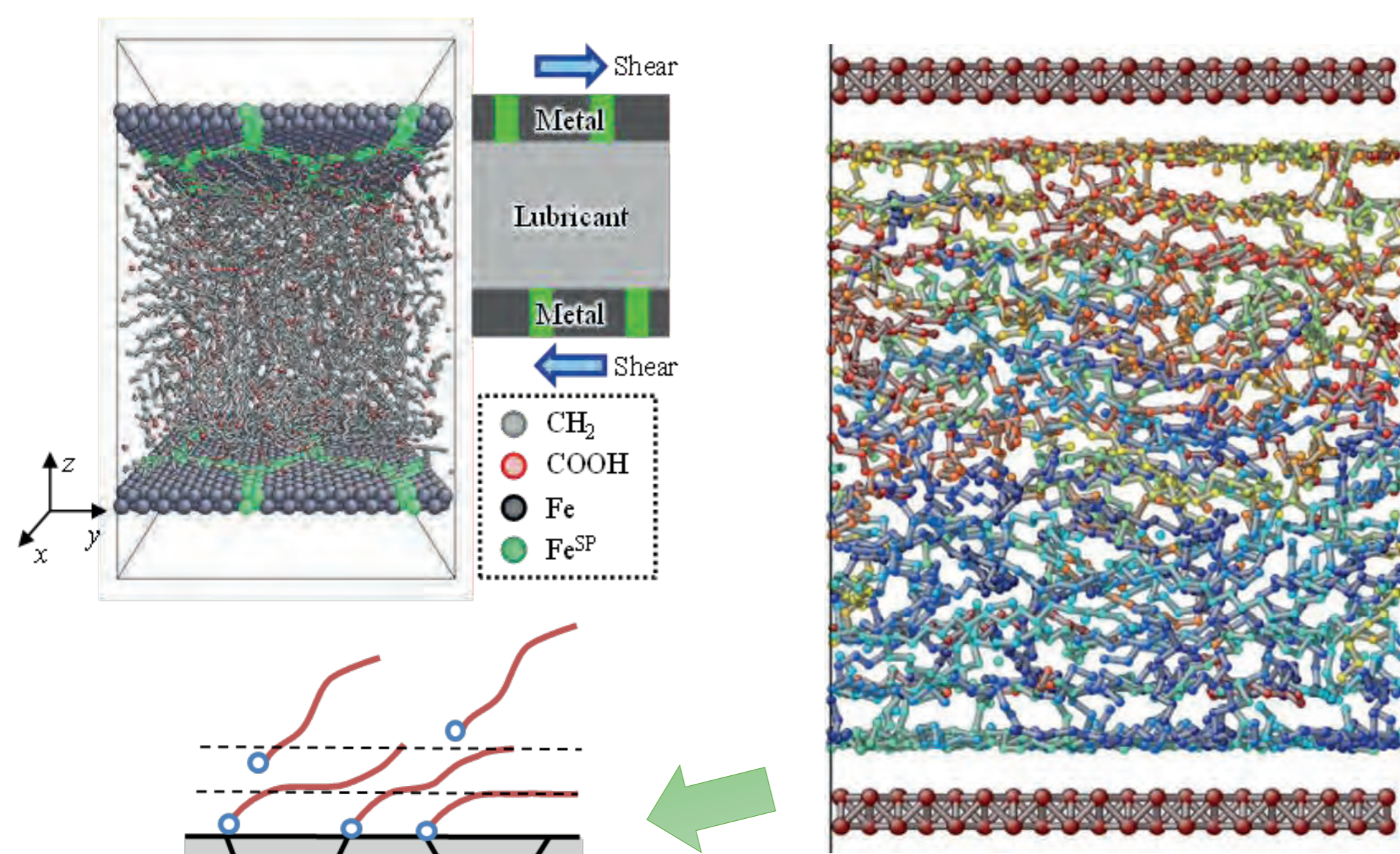


Atomistic model analysis of buckling behavior of carbon nanotubes under axial compression



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

