Theoretical Prediction of Strength and Physics of Nanomaterials 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.

**Effect of normal stress on ideal shear strength**

Ideal shear stress (ISS) under compression/tension, which is important to interpret experiments (e.g., nano-indentation tests), has been calculated. Response of ISS qualitatively differs. Note that compression always increases ISS in metals.

**Compression of carbon nanotubes**

Analysis of band gap energy of carbon nanotubes under radial compression

Prediction of peculiar radial buckling under pressure (radial corrugation)

**Atomic structure instability analysis**

Instability mode analysis of dislocation initiation from defect.

**Multiscale simulation of polymer materials**

Isotropic tension

Biaxial tension

Coarse-grained MD simulation

FEM analysis of crack propagation