Umeno Lab.

[Atomistic and electronic modeling analysis of strength and physical properties of solids]

Department of Fundamental Engineering

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

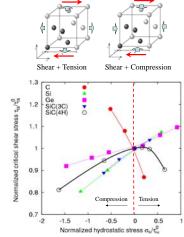
Computational Materials Science and Mechanics

Dept. of Mechanical Engineering

Toward Theoretical Prediction of Strength and Physical Properties of Nanomaterials

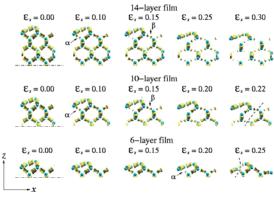
With the aim to reveal fundamentals of the mechanical and physical properties of nanomaterials, we are performing ab initio density functional theory calculations and molecular dynamics simulations.

Effect of normal stress on ideal shear strength



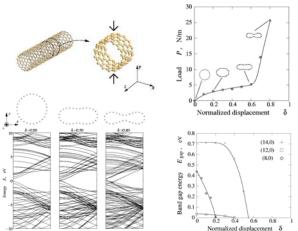
Ideal shear stress (ISS) under compression/tension, which is important to interpret experiments (e.g. nano-indentation tests), has been calculated. Response of ISS qualitatively differs. Note that compression always increases ISS in metals

Fracture of Si nanofilms under tension



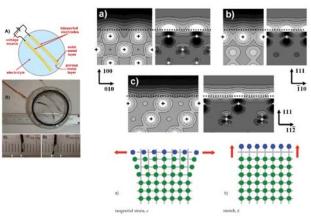
Deformation and fracture of Si nano-films were evaluated by DFT.

Compression of carbon nanotubes



Mechanical properties and band gap of carbon nanotubes under radial compression have been evaluated. Compression can change electronic conductivity.

Deformation of nano-porous metals in electrolyte



Deformation mechanism of nano-porous metal actuators has been theoretically revealed; i.e., how electric field can change surface stress.