

# Umeno Lab.

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

Center for Research on Innovative Simulation Software

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

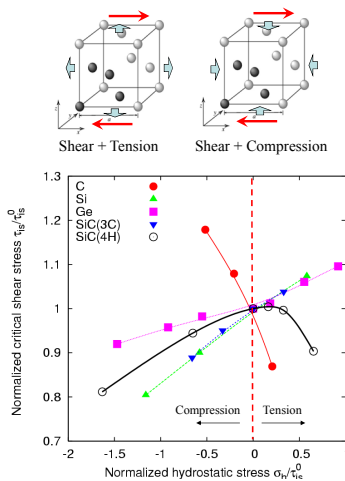
Nanostructured Materials Strength and Science

Dept. of Mechanical Engineering

## Toward Theoretical Prediction of Strength and Physical Properties of Nanomaterials

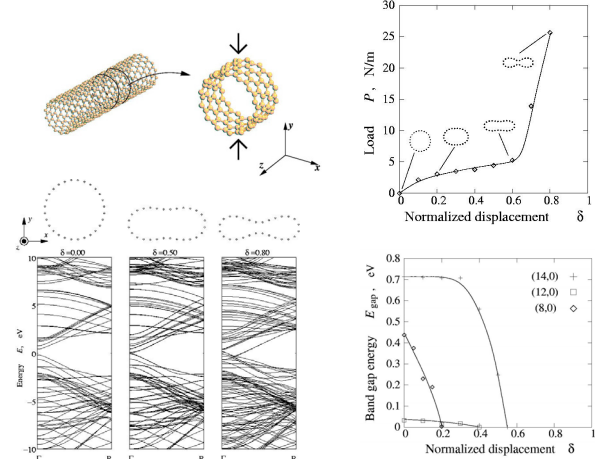
With the aim to reveal fundamentals of the mechanical and physical properties of nanomaterials, we are performing ab initio density functional theory calculations and molecular dynamics simulations.

### Effect of normal stress on ideal shear strength



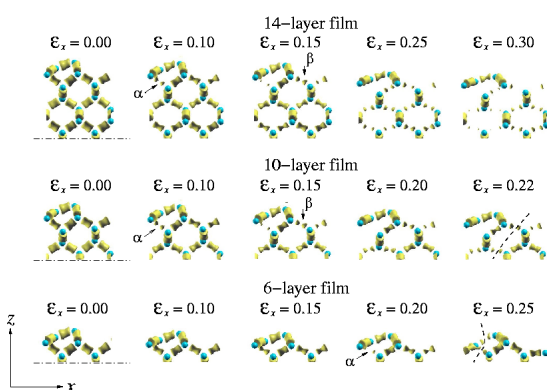
Ideal shear stress (ISS) under compression/tension, which is important to interpret experiments (e.g. nano-indentation tests), has been calculated. Response of ISS qualitatively differs. Note that compression always increases ISS in metals.

### Compression of carbon nanotubes



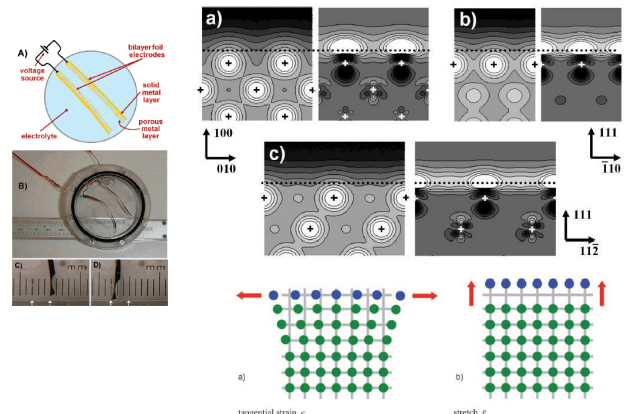
Mechanical properties and band gap of carbon nanotubes under radial compression have been evaluated. Compression can change electronic conductivity.

### Fracture of Si nanofilms under tension



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

### 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.