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

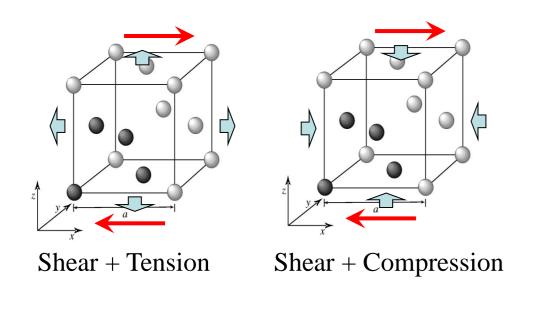
Nanostructured Materials Strength and Science

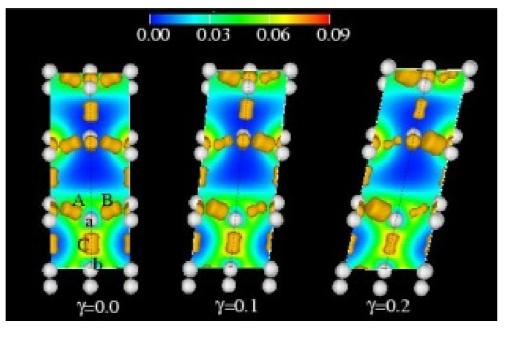
Dept. of Mechanical Engineering

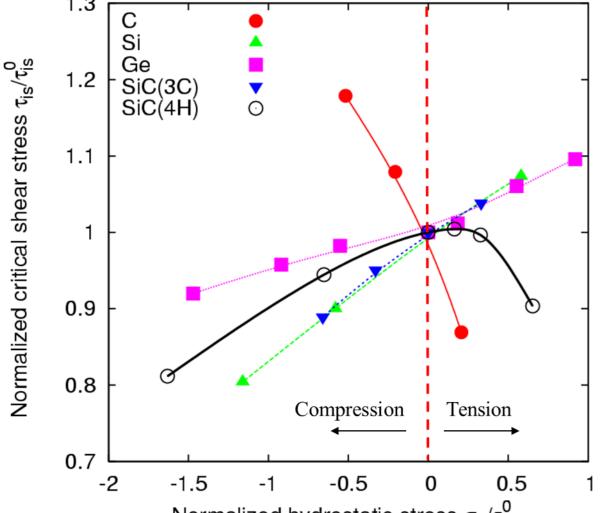
Toward Theoretical Prediction of Strength and Physical Properties of Nanomaterials

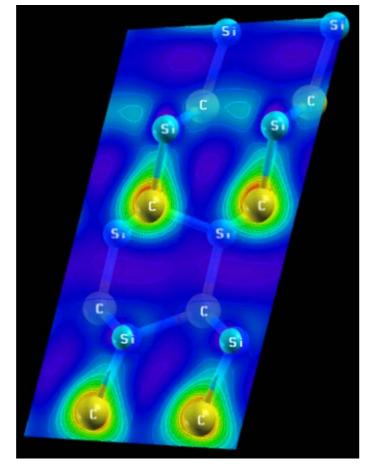
With the aim to reveal fundamentals of the mechanical and physical properties of nanomaterials, we are performing ab initio density functional theory calculations and molecular dynamics simulations.

Effect of normal stress on ideal shear strength



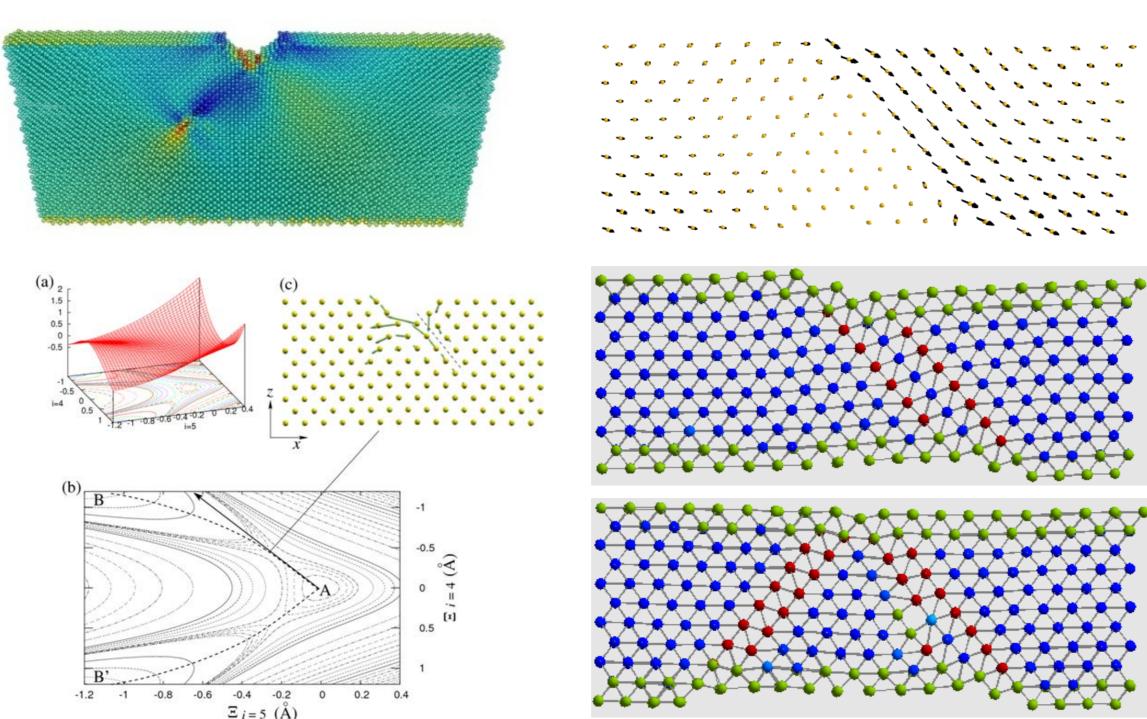






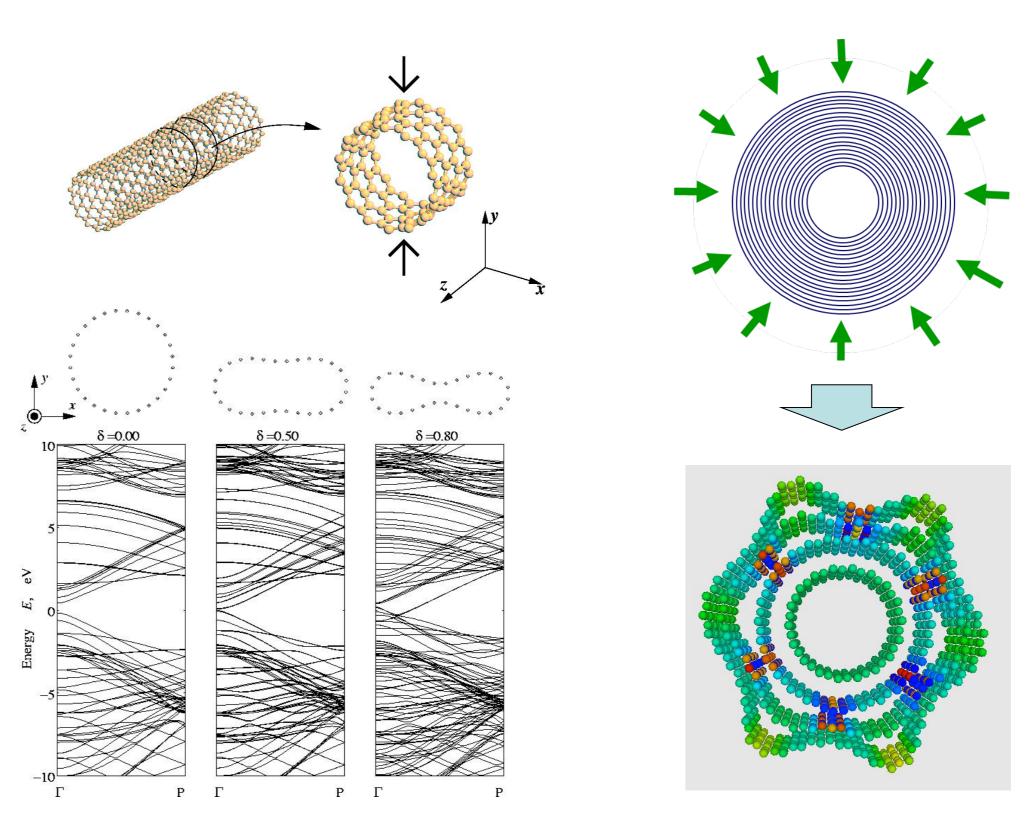
Normalized hydrostatic stress σ_h/τ_{is}^0 Ideal shear stress (ISS) under compression/tension, which is important to interpret experiments (e.g. nanoindentation tests), has been calculated. Response of ISS qualitatively differs. Note that compression always increases ISS in metals.

Atomic structure instability analysis



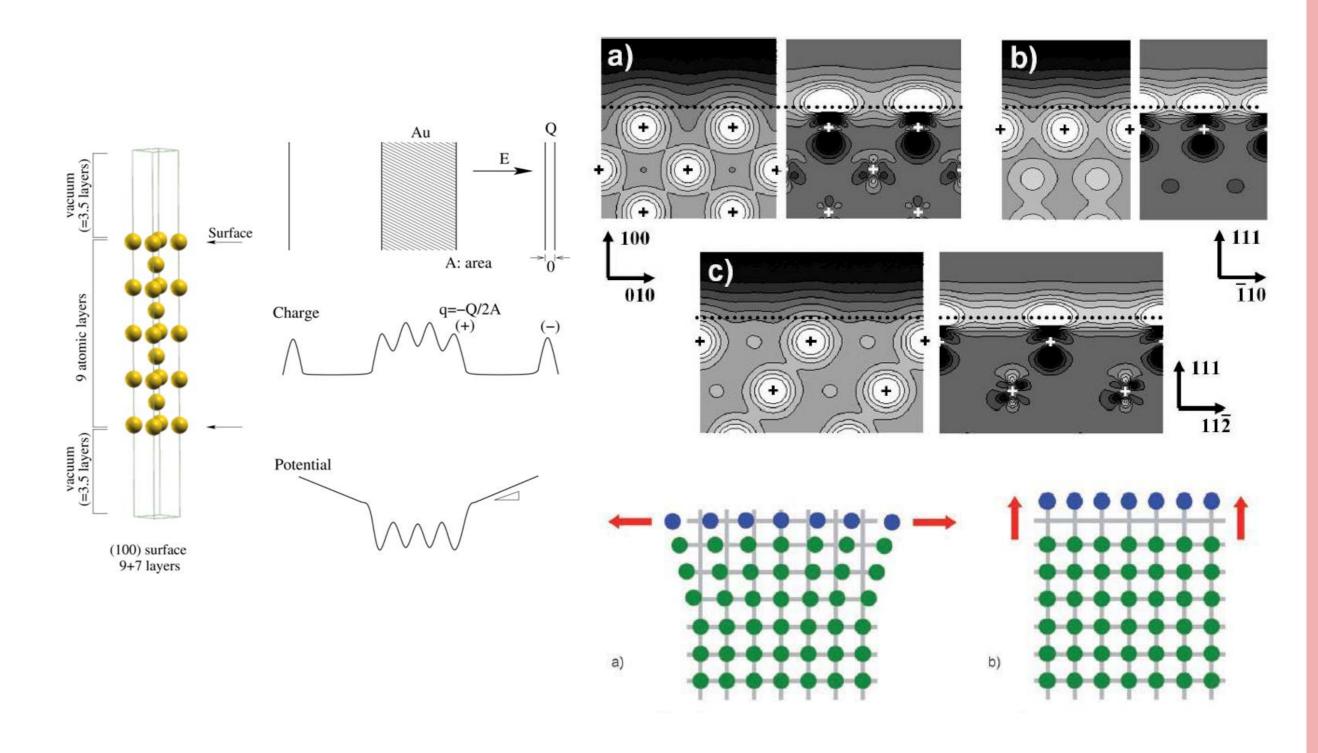
Instability mode analysis of dislocation initiation from defect.

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.