UMENO LAB. [Multiscale Simulation of Strength and Property of Materials]

Center for Research on Innovative Simulation Software

Nanostructured Materials Strength and Science

Dept. of Mechanical Engineering

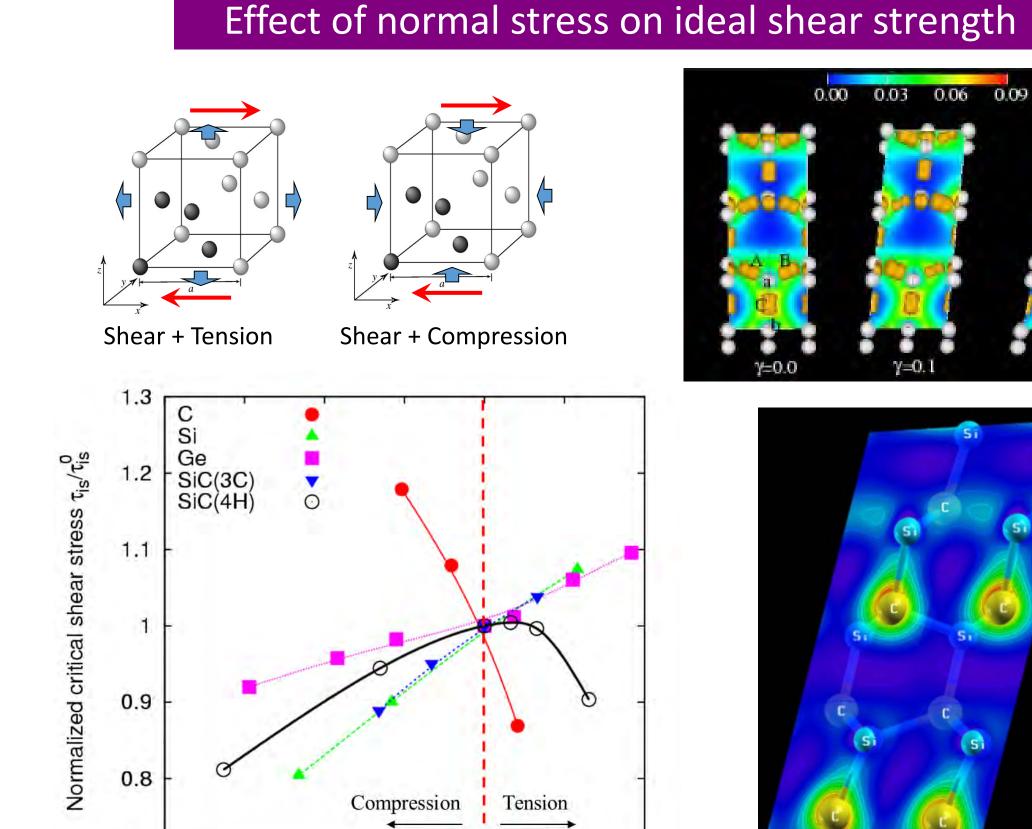
CISS

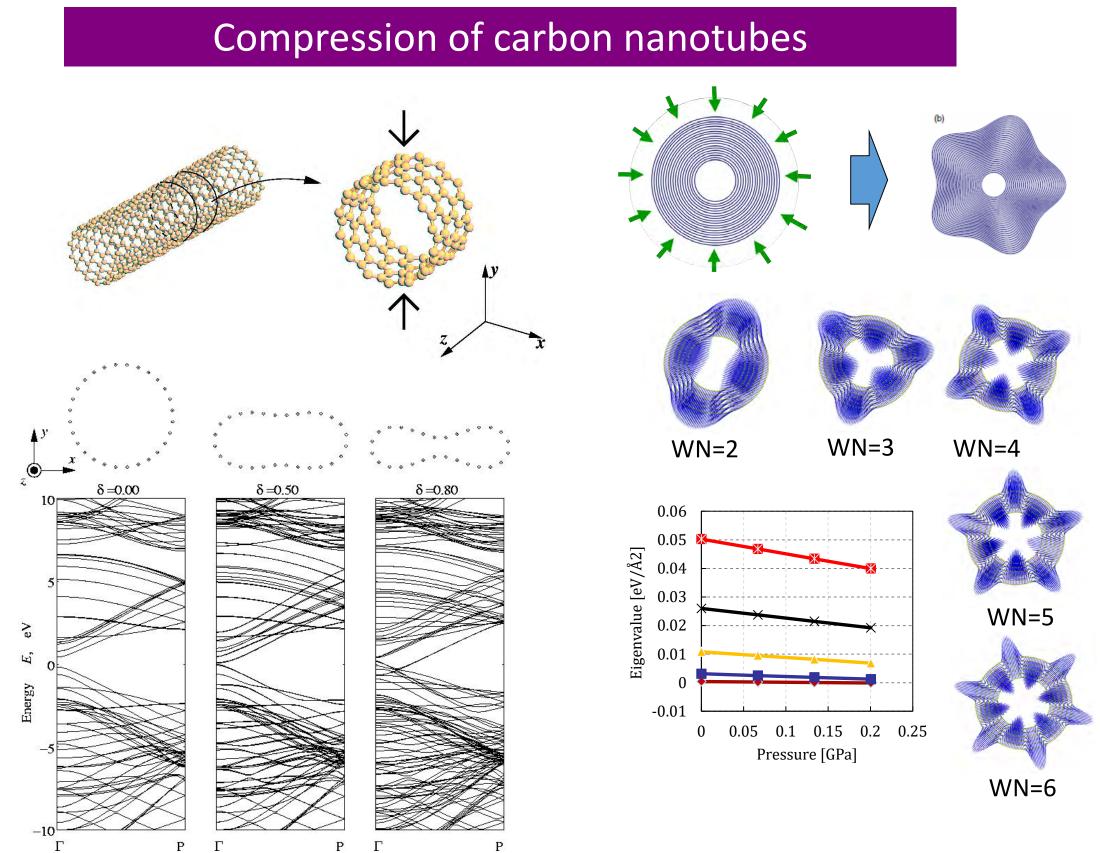
http://www.cmsm.iis.u-tokyo.ac.jp

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.



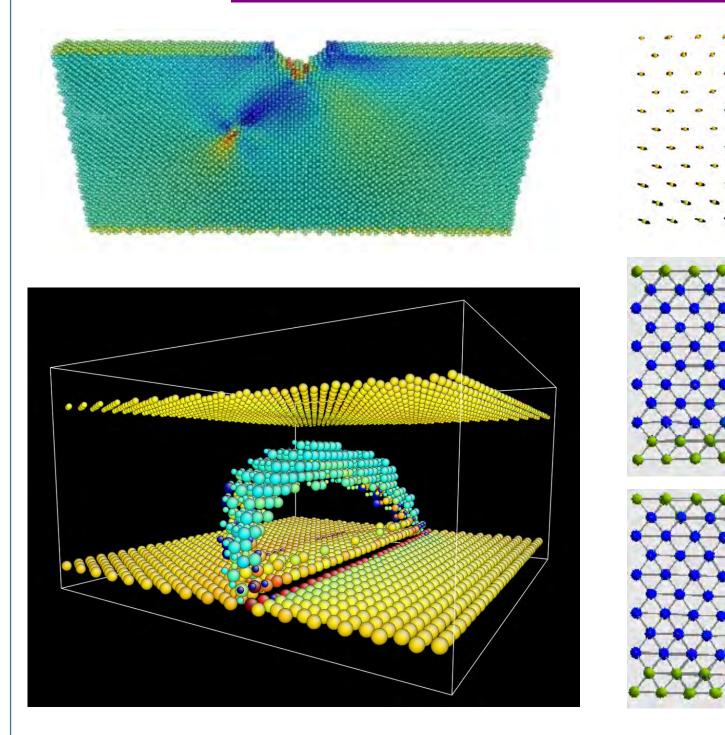


0.7 -2 -1.5 -1 -0.5 0 0.5 Normalized hydrostatic stress $\sigma_{\rm h}/\tau_{\rm is}^0$



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.

Atomic structure instability analysis



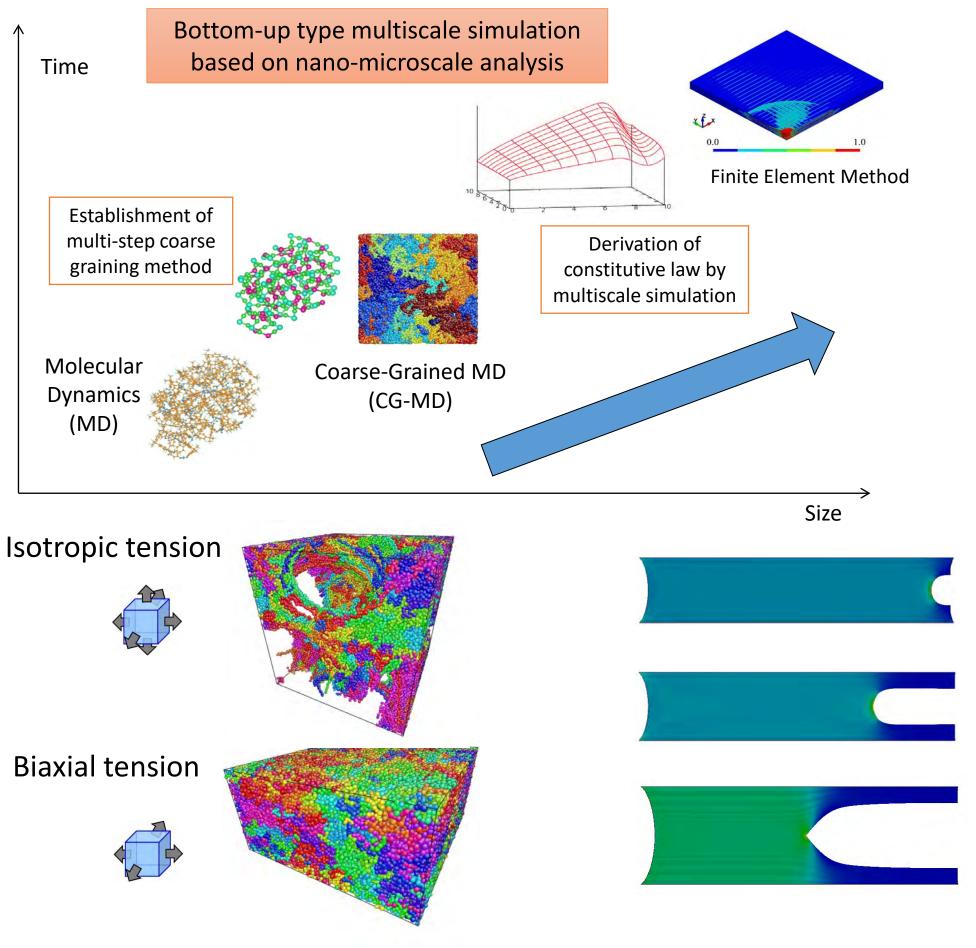
Molecular dynamics simulation of dislocation emission from defects

Instability mode analysis of dislocation initiation from defect

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Analysis of band gap energy of carbon nanotubes under radial compression Prediction of peculiar radial buckling under pressure (radial corrugation)

Multiscale simulation of polymer materials



Coarse-grained MD simulation

FEM analysis of crack propagation



