Research topics for graduate students for 2025

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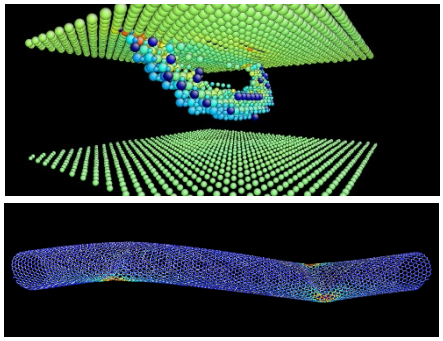
Acceptable course(s)

- Master's Degree
- Doctoral Degree

Research Topics



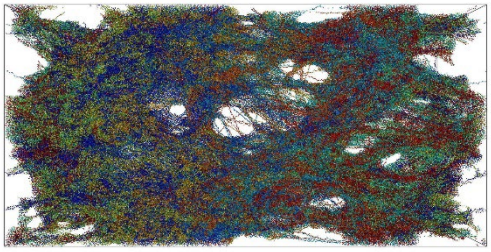
We are performing multiscale modeling and simulation of various materials, mainly focusing on their mechanical behaviors such as deformation and fracture but also investigating other physical properties. Our simulation methods include the first-principles density functional theory, all-atom and coarse-grained molecular dynamics, the phase field method and the finite element method.

1. Buckling behavior of carbon nanotubes

Electronic structures of carbon nanotubes can be modulated by the application of deformation. Such an effect can be utilized to fabricate novel nano-devices. In particular, carbon nanotubes can exhibit buckling deformation under compressive loads. Utilizing large and sudden change in the atomistic structure associated with buckling may pave the way for new nano-devices where abrupt and eminent modulation of electronic properties such as band-gap energy is expected with small input of mechanical loading. We perform molecular dynamics simulations and electronic structure calculations to clarify the mechanical and physical behaviors of carbon nanostructures.

2. Multiscale simulation of structural polymer materials and composites

As the application of plastic composite materials to automobiles and airplanes is getting more and more accelerated these days, it is urged to establish guidelines for designing polymer materials possessing both high strength and toughness. We perform multi-scale simulation aided by all-atom and coarse-grained molecular dynamics to obtain constitutive laws of materials and finite-element method (FEM) simulations to reproduce deformation and fracture in polymers.



3. Multiscale simulation of nano-micro fatigue

Fatigue of materials is a phenomenon that arises when the materials are under cyclic load, leading to crack initiation, crack propagation and fracture. Despite its industrial importance and also scientific profoundness, microscopic mechanisms of fatigue crack initiation have been little understood. We are working on the development of a novel multiscale simulation method to elucidate fatigue mechanisms at the nano and micrometer scales. Utilizing machine-learning, the new method combines deductive (bottom-up) and inductive (top-down) multiscale approaches, by which one can perform multiscale simulations overcoming drawbacks of both the conventional schemes.

Lab. Web page: http://www.cmsm.iis.u-tokyo.ac.jp/en/

YouTube channel: https://bit.ly/3wp6XAI