Lecture 3: Continuous vs. Discrete Systems, Equations of Motion

January 18, 2010

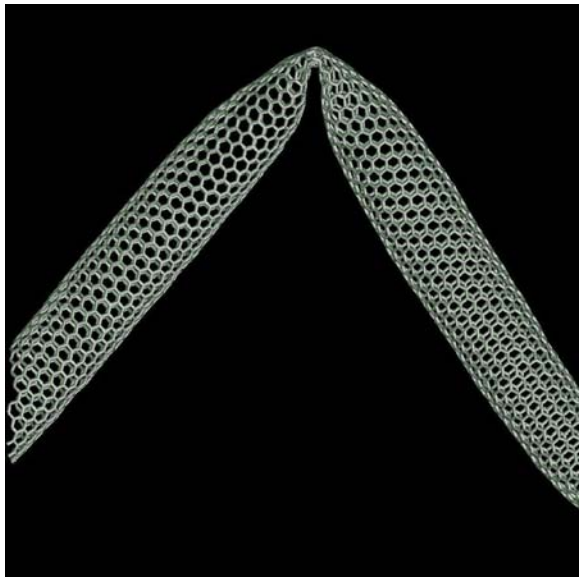
Outline

- Continuous vs. discrete systems.
- Purpose of MD and some applications.
- Equations of motion: formulation and discretization.

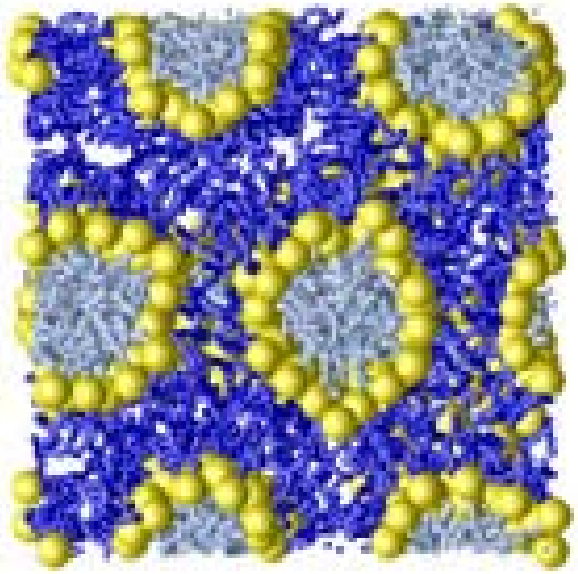
MD Simulations

- In an MD simulation, the time histories of the positions and momenta of a set of particles are predicted using Newton's 2nd law.
- Can make atomic level observations not possible in experiments.
- From these position and momenta, we can calculate/predict quantities such as energy, temperature, pressure, thermal conductivity, viscosity, …
- In a non-equilibrium simulation, can observe a process (fracture, reaction, phase change, …)

Examples

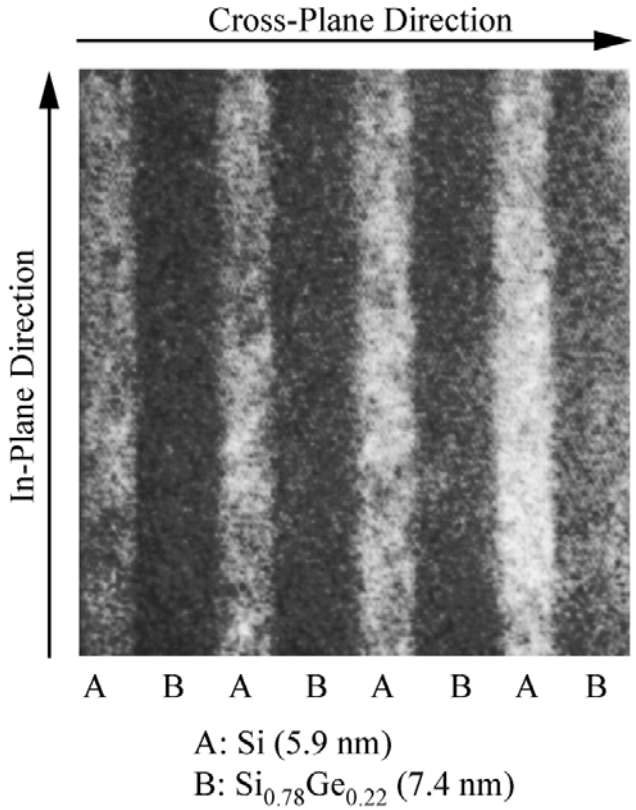


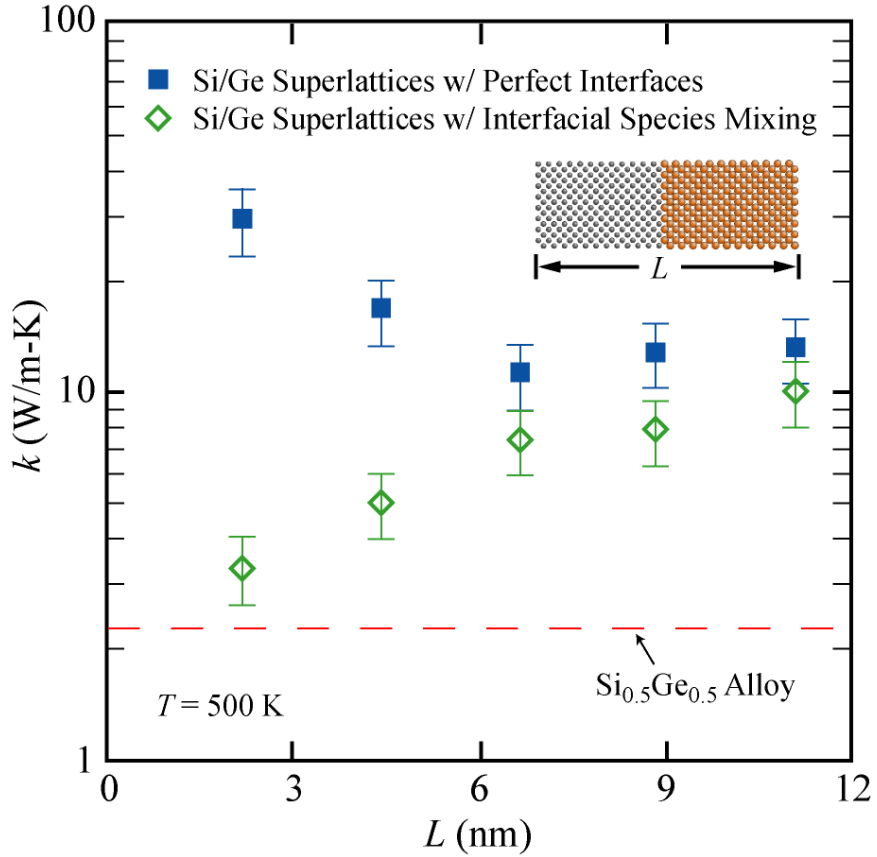
Bending of a carbon nanotube
J. Li, OSU

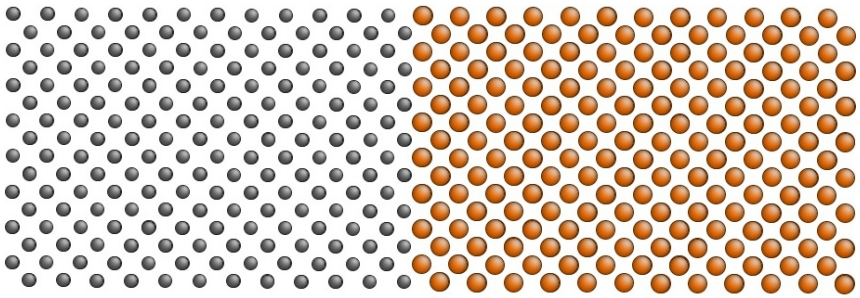


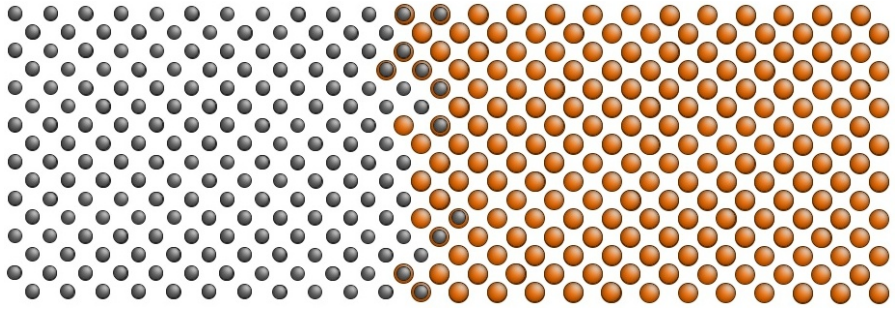
Assembly of tethered nanoparticles,
S. Glotzer, UM

Heat Transfer in Superlattices









Landry and McGaughey, *Physical Review B* **79** (2009) 075316.