MSE 165/175: Nanoscale materials physics computation laboratory
Evan Reed, Winter Quarter 2014

Course description:
Computational exploration of fundamental topics in materials science using interactive Java-based computation and visualization tools. Emphasis is on the atomic-scale origins of macroscopic materials phenomena. Simulation methods include molecular dynamics and Monte Carlo with applications in thermodynamics, statistical mechanics, kinetics, material imperfections, mechanical properties, mechanical response. Recommended prerequisites: Some very basic programming skills.

Textbooks:
- Thermal and Statistical Physics by Gould and Tobochnik
  - Available electronically at: http://stp.clarku.edu/notes/
- Materials Science and Engineering: An Introduction by Callister (8th Ed.)
- There is no text at the bookstore for this class

Syllabus:
- Atomic (molecular) dynamics and Monte Carlo methods
- Atomic origins of temperature, entropy
- Microcanonical, canonical ensembles
- Magnetism and lattice gas using Ising model
- Phase diagrams: Monatomic substance and binary alloy
- Phase transitions: Kinetics, nucleation and growth, spinodal decomposition
- Material imperfections: Vacancies, dislocations, cracks, grain boundaries
- Mechanical properties of materials: Fracture mechanics, brittle and ductile failure, crack propagation