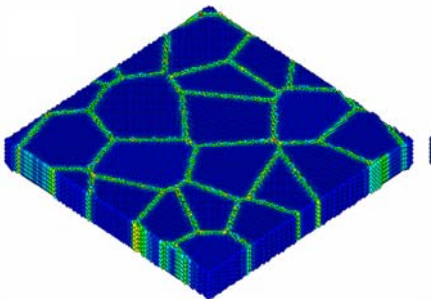
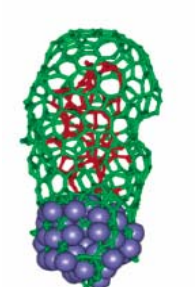
MEEG 591 – Multiscale Modeling
Spring 2008

Instructor: Dr. Douglas Spearot, MEEG 103, 575-3040, dspearot@uark.edu
Lecture: Monday/Wednesday/Friday, 8:30 – 9:20 am
Classroom: MEEG 101

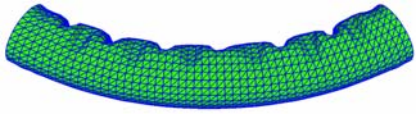
Course Objectives: To provide the student with an overview of different modeling techniques in materials science. Applications will be presented that utilize computational tools to study the structural, mechanical, chemical and electrical properties of materials. A broad range of modeling techniques will be covered that span from quantum to continuum domains. Particular focus will be given to "atomistic" modeling techniques, including molecular mechanics, molecular dynamics and Monte Carlo simulations.



Nanocrystalline Materials



Carbon Nanotube Synthesis



Carbon Nanotube Mechanics

Course Topics:

1) Introduction to Numerical Simulation
   a) What is computational materials science? (1 lecture)
   b) Length and time scale considerations (1)
2) Atomistic simulations
   a) Basic principles – Thermodynamic properties / Ensembles (3)
   b) Interatomic potentials (4)
   c) Molecular mechanics (4)
   d) Molecular dynamics (6)
   e) Monte Carlo methods (3)
3) Overview of finite element methods (3)
4) Coupling methods between atomistics and finite elements
   a) Concurrent coupling versus hierarchical coupling (1)
   b) Hierarchical coupling (2)
   c) Concurrent coupling – Cauchy Born rule, Quasicontinuum, etc. (3)
5) Project Presentations (5)

Homework: Homework will be assigned and collected as necessary over the course of the semester. No late homework assignments will be accepted without prior approval.

Project: Students will be required to complete a course project. Students will be asked to present the results of their work via a written report and an oral presentation (during the regular class period). The course project does not require computer programming.

Grading: Final Project 66%, Homework 34%