

EE582 sec. 3

Special Topics  
Molecular Simulations of Nanostructures  
Spring 2006

Schedule Line #: 74310

Time and Place: TU,TH9:10-10:25 THOM 5

Course Description:

This course will cover the details of molecular dynamic approach and its applications to examine the material properties of nanoscale materials. Both MD algorithm and the physics of materials at nanoscale will be discussed. The class will involve hands-on experience on using classical MD simulations to investigate material properties such as thermal and mechanical properties (stress and strain) and effects of defects.

Topics:

1. Molecular Dynamic Approach:
2. Intermolecular Forces and Potentials fields
3. Equilibrium and non-equilibrium MD approach
4. Calculation of Transport Coefficients.
5. Physics of Linear atomic chains, two and three dimensional crystals
6. Properties of Phonon gas
7. MD simulation of microscale heat transfer
8. Stress and strain
9. Carbon Nanotubes and Diamondoids
10. Electronic properties and quantum MD.

Text Books:

1. [The Art of Molecular Dynamics Simulation](#) (2nd Edition)  
D. C. Rapaport (examples in C ).  
ISBN: 0521-82568-7 (Hardback), Cambridge University Press, 2004
2. Foundations of Nanomechanics  
A.N. Cleland  
ISBN 3-540-43661-8  
Springer-Verlag 2003

Other books;:

1. "Understanding Molecular Simulation", D. Frenkel and B. Smit, 2<sup>nd</sup> edition, Academic Press, 2002, ISBN: 0-12-267351-4 (examples in Fortran)
2. *Molecular Dynamics*, Wm. G. Hoover, Springer Verlag, 1986.

Handouts and material from the internet will be used to supplement the text books.

Other recommended reading material:

<http://www.mse.ncsu.edu/CompMatSci/Tutorial/>

<http://www.photon.t.u-tokyo.ac.jp/~maruyama/papers/02/HEDU.pdf>

<http://www.photon.t.u-tokyo.ac.jp/~maruyama/mdlecture/advances.pdf>

Grading:

Homework	20%
Project	40%
Midterm examination	40%