Introduction of computational methods applied to nuclear materials, ranging from atomic-level simulations to mesoscale technique to continuum modeling. Topics covered include radiation damage, ion-solid interaction, and microstructure evolution, and defect interactions with grain boundaries, dislocations and precipitates. Also, state-of-the-art of computational approaches to study microstructural evolution in nuclear materials will be discussed.  The subject matter may change from term to term.

1/20 Introduction

Challenges for Computational Nuclear Materials

Nuclear material Issues, Radiation Damage, Multi-Scale Computer Simulation, Various Simulation Methods, Applications of Computer Simulations and Prediction of Materials Properties

1/25 – 1/27 Basic Knowledge of Computational Materials – I, II

Material Structures, Material Types, 1D, 2D and 3D Lattices, Miller Indices, Interstitials, Formation of Defects, Phase Transformation and Radial Distribution Function

2/1 Basic Knowledge of Computational Materials III

Forces and Cohesive energy, Bonding, Covalent, Ionic and Metallic Materials, Interatomic Potentials and Molecular Crystals

2/3 Lab. Exercise

Crystal Structures and Defect Visualization

2/8

First Principle Calculation and Analysis of Results

Electronic Structure, Use of Quantum Code, Magnetism, Density of States, Charge Density

2/15 Density Functional Theory (DFT)

DFT and Many-Body Interaction, Self-Consistent Computational Approach

Quantum molecular dynamics

Local Density Approximation (LDA), [Generalized Gradient ApproximationLinks to an external site.](http://www.google.com/url?sa=t&rct=j&q=&esrc=s&source=web&cd=1&ved=0CB4QFjAA&url=http%3A%2F%2Farxiv.org%2Fabs%2F1305.0108&ei=d9yqVMW6FMWtU-jxgKAL&usg=AFQjCNEtcTBb8UH3B8r2PCg18eiXCSfBLw&sig2=dgiDHTIT17I6HNPnmHoZdw&bvm=bv.82001339,d.d24)(GGA)

Applications to Defect Calculations

2/17 DFT Lab with Different Codes

Calculate Defect Configurations

Determine Formation Energies of Defects in BCC and FCC Materials

Impurities in Materials

2/22-2/24 Interatomic Potentials

Concept of Interatomic Potentials, Pair Potentials, Empirical Interatomic Potentials for Metals, Potentials for Covalent and Ionic Materials, Development of Interatomic Potentials, Advantages and Disadvantages of Various Interatomic Potentials

3/1 Lab work on Interatomic Potentials

Visualization of Interatomic Potentials, Pair Potentials, Empirical Interatomic Potentials for Metals, Formation and Binding Energies of Defects

3/3-3/8 Energy and Geometry Optimization Methods

Energy Evaluation, Steepest Descents, Newton-Raphson,Conjugate Gradient

Simulated Annealing

Defect Configuration, Formation and Defect Cluster Optimization

3/10 Lab Work on Energy and Geometry Optimization of Defects and Defect Clusters

3/15 Midterm Exam

3/17 – 3/22 Molecular Dynamics (MD) Method

Basics of MD, Periodic Boundary Condition, Velocity rescaling, Temperature Control, Different Ensembles

MD in Nuclear Materials

3/24  Lab Work on MD Simulations

Diffusion of Defects, Defect Generation and Defect Interaction

3/29 – 3/31 Monte Carlo (MC) Method

Random Number and Probability, Metropolis Algorithm, Kinetic Monte Carlo Method, Time in A MC Simulation, MC Against MD, Applications of MC to Nuclear Materials (Diffusion, Defect Accumulation, Defect Interaction with Microstructures)

4/5 Lab Work on MC Simulations

Random Number Generation, Defect Diffusion, Defect Annealing and Defect Accumulation

4/7-4/12 Phase Field Model and Simulation

Free-Energy Functional, Elastic Energy, Phase Field Model, Microstructure Evolution, Applications of Phase Field Model to Nuclear Materials (Phase Segregation, Growth of Dislocation Loops, Gas Bubble Evolution)

4/14-4/19 Rate Theory, Cluster Dynamics, Dislocation Dynamics

Basics and Introduction of Rate Theory, Dislocation Dynamics, Cluster Dynamics

Applications to Nuclear Materials

4/21-4/26 Project Presentation

**Grading**:

Homework and Lab Work:     50 %

Midterm exam: March. 15      20 %

Final Project: April 21-26      30 %

**Text Book (optional)**: **Introduction to Computational Materials Science by Richard Lesar (Cambridge University Press, 2013)**

**Reference**:

1. 1. **A. R. Leach, *Molecular Modelling: Principles and Applications*, (Pearson Education Press, 2001).**
2. **E. Kaxiras, *Atomic and Electronic Structure of Solids*, (Cambridge University Press, 2003).**
3. **R. M. Martin, *Electronic Structure*, (Cambridge University Press, 2004).**
4. **K. Ohno, K. Esfarjani, K. Kawazoe, *Computational Materials Science*, (Springer, 1999).**
5. **Allen and Tildesley, *Computer Simulations of Liquids*, (Oxford University Press, 1986).**
6. **M. Finnis, *Interatomic Forces in Condensed Matter*, (Oxford University Press, 2003).**