Department of Scientific Computing
College of Arts and Science
Florida State University

ISC 5934(4): Computational Materials Science

(spring 2010)

Professor Anter El-Azab

Place/Time Tuesday, Thursday 12:30–1:45 pm
Room DSL 468

Office hours: Monday 10:00 am–12:00 noon
(and whenever I am in office)
DSL 415 (my office)

Contact information

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Grading

- Homework 25%
- Midterm 25% (can be a take-home test)
- Term project 25%
- Final exam 25% (can be a take-home test)

- Midterm will be given in the 8th week (tentatively). Exact date will be fixed later.

- Final exam time/place, per FSU exam schedule.

- Homework is due a week from the date it is assigned (about 6-8 assignments will be given).

- See project details later in this document.

… remarks

- Expect high level theoretical concepts
- Take class seriously – this is the only opportunity to see this part of the field of materials science at FSU
- Please interact in class and participate in discussion
- Set ambitious learning goals for this course
- Try to connect the concepts and ideas of this class to your research
- Do extra free reading related to the subject (project)
- Return assignments on time

FSU Policy statement

- The Florida State University Academic Honor Policy outlines the University's expectations for the integrity of students' academic work, the procedures for resolving alleged violations of those expectations, and the rights and responsibilities of students and faculty members throughout the process. Students are responsible for reading the Academic Honor Policy and for living up to their pledge to "... be honest and truthful and ... [to] strive for personal and institutional integrity at Florida State University." (Florida State University Academic Honor Policy, found at http://dof.fsu.edu/honorpolicy.htm.)

AMERICANS WITH DISABILITIES ACT:

- Students with disabilities needing academic accommodation should:
(1) register with and provide documentation to the Student Disability Resource Center; and
(2) bring a letter to the instructor indicating the need for accommodation and what type. This should be done during the first week of class.

- This syllabus and other class materials are available in alternative format upon request.

- For more information about services available to FSU students with disabilities, contact the:
Student Disability Resource Center
874 Traditions Way
108 Student Services Building
Florida State University
Tallahassee, FL 32306-4167
(850) 644-9566 (voice)
(850) 644-8504 (TDD)
sdrc@admin.fsu.edu
http://www.disabilitycenter.fsu.edu/

Catalogue description

ISC 5935(4): Computational Materials Science (3). Fundamentals of materials defects at the atomic and microstructural scales, statistical theory of defects, elastic models of materials defects, diffusion, thermodynamics and kinetics in defect disordered solids, phase changes, and microstructure evolution in materials. Monte Carlo and Phase Field methods will be used for computational illustration of various aspects of defect dynamics and microstructure evolution.

Course objectives (student learning)

At the end of the course, the students will be able to

- model the elastic and statistical properties of defects,
- simulate and model diffusion of atomic defects in materials,
- conduct quantitative modeling of nucleation, growth and coarsening in materials,
- construct models of microstructure evolution in materials and study the motion of grain boundaries and interfaces,
- use Monte Carlo method in modeling thermodynamics and kinetics of defects in materials, and
- develop and use phase field models to study compositional and phase changes and growth in materials.

Prerequisites

- Basic knowledge of atomic structure of materials
- Basic concepts of continuum mechanics
- Graduate standing in engineering mathematics and/or mathematical physics
- Some background in statistical mechanics or molecular mechanics should be helpful

Topics covered (coarse description)

- Defects in materials (point defects, dislocations, grain boundaries, ...)
- thermodynamics of defects,
- atomic and defect diffusion in materials,
- aspects of compositional and phase changes in materials,
- aspects of microstructure evolution in materials, and
- computational methods (Monte Carlo, Phase Field methods).

Syllabus details

Part I: Defects in Materials

- Point defects in crystalline materials
- Defects production in irradiated materials
- Dislocations
- Elastic models of defects
- Structure of grain boundaries
- Surfaces and interfaces
- Heterogeneity in materials

Part II: Thermodynamics of Defects

- First and second laws of thermodynamics
- Free energy of defect-disordered materials (pure metals, alloys, ordered materials)
- Statistical models of free energy
- Elastic and interfacial energy of extended defects
- Free energy of materials with multiple types of defects
- Order parameters in materials

Part III: Atomic and Defect Diffusion in Materials

- Diffusion mechanisms
- Phenomenological theory of diffusion
- Computational modeling of diffusion
- Surface diffusion

Part IV: Aspects of Compositional and Phase Changes in Materials

- Segregation in metals and oxide systems
- Nucleation theory
- Growth and coarsening kinetics
- Spinodal decomposition

Part V: Aspects of Microstructure Evolution in Materials

- Concept of materials forces (force on defects)
- Mechanisms of grain boundary motion
- Domain boundary motion
- Dislocation dynamics
- Morphological evolution of crystals and thin films

Part VI: Computational Methods

- Monte Carlo simulations in thermodynamics and kinetics of materials
- Phase field modeling of phase changes, morphological evolution and microstructure changes

Projects

Following the introductory part of the course, sample projects will be discussed in class and each student or two will select one project. The students will conduct guided reading on this project area for three weeks at the end of which, and based on consultation with the instructor, the students will identify project problems to work on. The project work involves literature assessment, mathematical modeling and computational implementation of a material problem, a written report not exceeding 10 pages, and a final presentation at the last class meeting.

Reference material

- Instructor's handouts, review articles, chapters, …
- Helmut Mehrer, Diffusion in Solids:Fundamentals, Methods, Materials, Difusion-Controlled Processes, Springer-Verlag Berlin Heidelberg 2007
- Martin Glicksman, Diffusion in Solids: Field Theory, Solid-State Principles, and Applications, John Wiley & Sons, 2000
- Robert W. Balluffi, Samuel M. Allen and W. Craig Carter, Kinetics of Materials, John Wiley & Sons, 2005
- A. Pimpinelli and J. Villain, Physics of Crystal Growth, Cambridge, 1998
- Nasr M. Ghoniem and Daniel Walgraef, Instabilities and Self-Organization in Materials, Volume I: Fundamentals of Nanoscience, Volume II: Applications in Materials Design and Nanotechnology, Oxford University Press, 2008

General remarks on Materials Science

About the Field of Materials science

- The science of structure and properties of all materials (structural, functional, biological, etc.)

- Structure of materials
  - Atomic structure
  - Mesoscale (hierarchical) structure

- Properties of materials
  - The characteristics of materials response under various circumstance
  - This may include: mechanical, physical, chemical response

- Long ago: the field of materials Science was dominated by empirical research

- Theory then became important … Lately, computational methods became important part of theoretical materials science

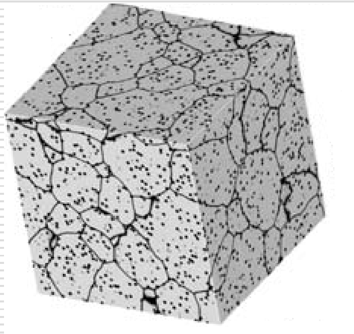
Different views of materials

- Physicists: order and symmetry, and consequences on properties of pure phases
- Chemists: chemical state (charge states) and reactivity
- Biologists: structure, reactivity, function
- Materials Scientists focus on microstructure. For the most part, the question of microstructure drives their thinking about materials because it is the key for processing and designing materials for various applications …

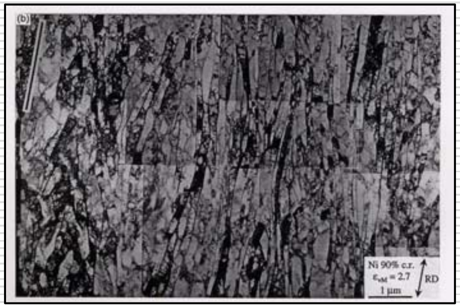
Microstructure materials

- The term microstructure refers to the geometrical aggregates of grains (units), phases, and structural defects
- Often materials exhibit complex microstructure
- Microstructure of materials evolves during processing (all about adjusting microstructure) and during utilization (aging of materials)

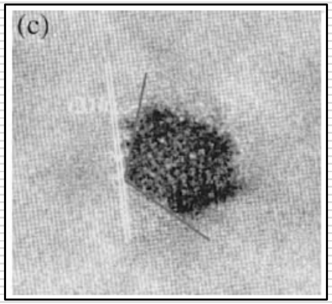
Example microstructures in materials



Grains in a polycrystalline material

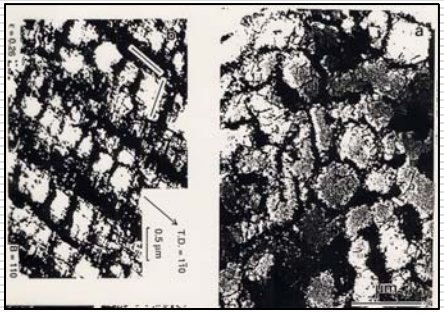


Sub-grain structure in rolled metals

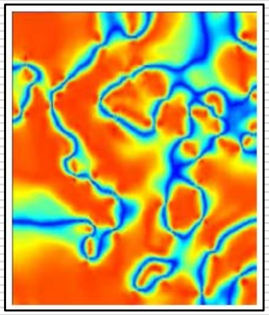


Precipitate in aluminum alloy

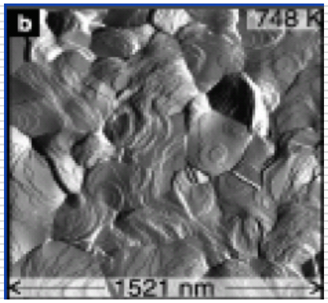
Example microstructures in materials



Dislocation microstructure in deformed metals

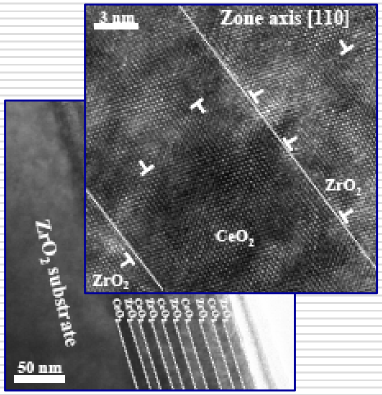


Ferroelectric domains



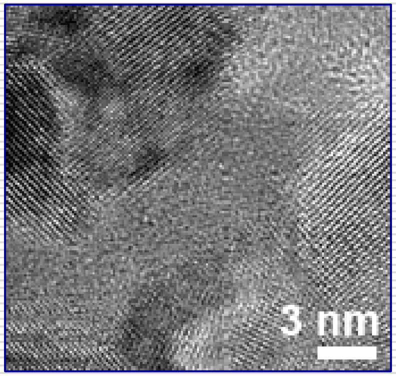
Polycrystalline gold film

Example microstructures in materials

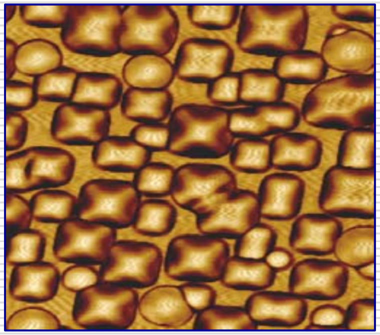


Oxide super-
lattice structure

(hetero-structure)



Amorphous/
crystalline
oxide

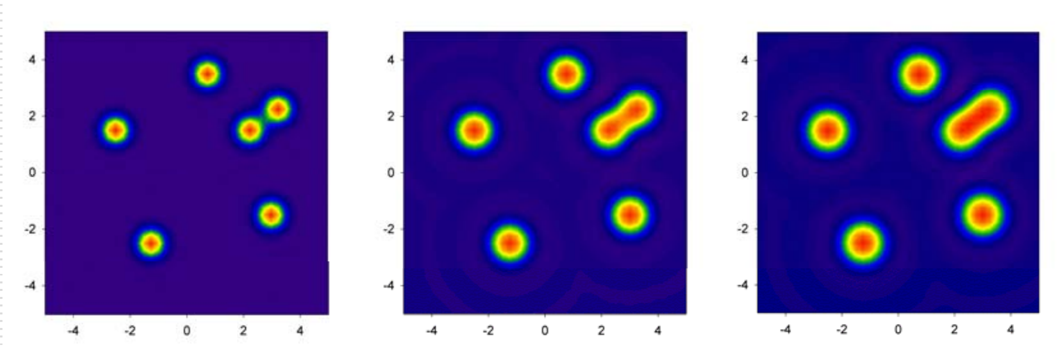


Quantum dot
structure

Microstructure evolution

- Microstructures change when materials are subjected to external drivers (mechanical forces, electric and magnetic fields, chemically reactive agents, heating, irradiation, etc.)
- **This evolution is often complex and it takes place by diffusion of atoms, motion defects and interfaces, or by spontaneous phase changes**
- New microstructure often appears and some disappears, reappears, etc.

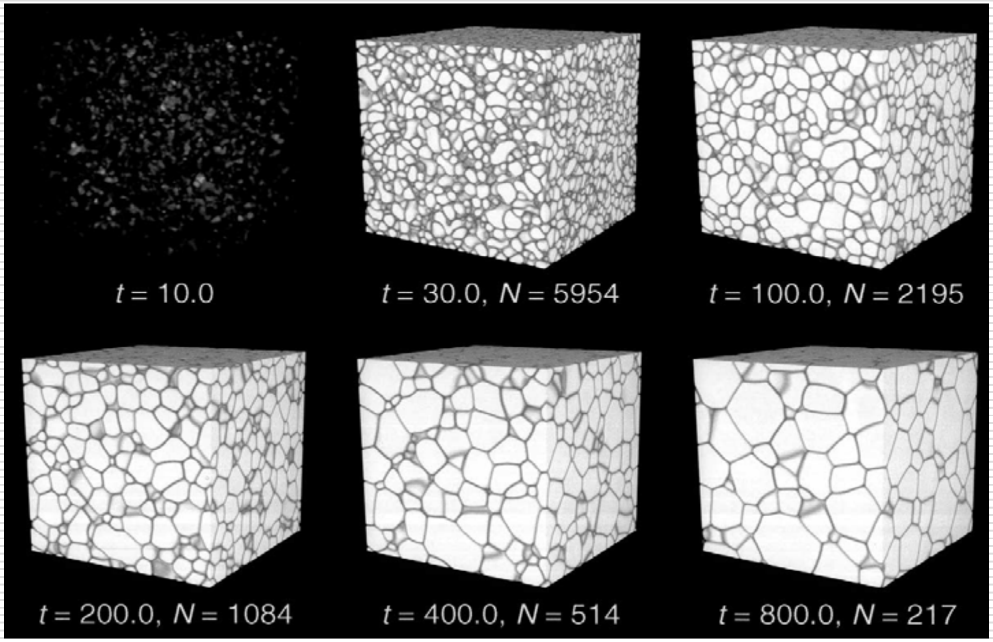
Microstructure evolution



Evolution of quantum dots on a surface

Evolution of dendrite structure during solidification

Microstructure evolution



Grain growth at elevated temperature