MSE 209: Introduction to the Science
and Engineering of Materials

Spring 2010  MSE 209 - Section 1
Instructor:  Leonid Zhigilei

Monday and Wednesday, 08:30 – 9:45 am
Olsson Hall 009
Research in Computational Materials Group:

Generation of crystal defects and melting in a metal target irradiated by a short laser pulse

Simulation of impact resistance of carbon nanotube materials

Temperature distribution in a simulation of heat transfer in a carbon nanotube material

Group Web Site: http://faculty.virginia.edu/CompMat/
Contact Information:

Instructor: Leonid Zhigilei
Office: Wilsdorf Hall, Room 303D
Office Hours: 10:00 am to 12:00 pm Tuesday & open
Telephone: (434) 243 3582
E-mail: lz2n@virginia.edu

Class web page:
http://www.people.virginia.edu/~lz2n/mse209/

Class e-mail list: 10f-mse-2090-1@collab.itc.virginia.edu

Graduate Teaching Assistant: Ms. Priya Ghatwai
Office: Materials Science Building 109
Office hours: 4-5 pm on Tuesdays and Wednesdays in Materials Science Building, Room 125A
You can also e-mail Ms. Ghatwai for additional appointments and individual consultations.
E-mail: pg9j@virginia.edu
Grading:

- Homework: 15%
- Two mid-term exams: 40%
- Final exam: 45%

Homework: 11 problem sets will be assigned and will be due at the beginning of class one week after assignment. Homework solutions should be neat and stapled. Homework does not require the pledge and cooperation among students is permitted. Copying is not permitted.

Late homework is not accepted

Tests: pledged, closed-book and closed-notes

Textbook:


I will also post my lecture notes on the web.
Syllabus:

- From atoms to microstructure: Interatomic bonding, structure of crystals, crystal defects, non-crystalline materials.

- Mass transfer and atomic mixing: Diffusion, kinetics of phase transformations.

- Mechanical properties, elastic and plastic deformation, dislocations and strengthening mechanisms, materials failure.

- Phase diagrams: Maps of equilibrium phases.

- Polymer structures, properties and applications of polymers.

- Electrical, thermal, magnetic, and optical properties of materials.
Chapter 1: Introduction

• Historical Perspective
  Stone → Bronze → Iron → Advanced materials

• What is Materials Science and Engineering?
  Processing → Structure → Properties → Performance

• Classification of Materials
  Metals, Ceramics, Polymers, Semiconductors

• Advanced Materials
  Electronic materials, superconductors, etc.

• Modern Material's Needs, Material of Future
  Biodegradable materials, Nanomaterials, “Smart” materials
Historical Perspective

- Beginning of the Material Science - People began to make tools from stone – Start of the Stone Age about two million years ago. Natural materials: stone, wood, clay, skins, etc.

- The Stone Age ended about 5000 years ago with introduction of Bronze in the Far East. Bronze is an alloy (a metal made up of more than one element), copper + < 25% of tin + other elements. Bronze: can be hammered or cast into a variety of shapes, can be made harder by alloying, corrode only slowly after a surface oxide film forms.

- The Iron Age began about 3000 years ago and continues today. Use of iron and steel, a stronger and cheaper material changed drastically daily life of a common person.

- Age of Advanced materials: throughout the Iron Age many new types of materials have been introduced (ceramic, semiconductors, polymers, composites…). Understanding of the relationship among structure, properties, processing, and performance of materials. Intelligent design of new materials.
A better understanding of structure-composition-properties relations has lead to a remarkable progress in properties of materials. Example is the dramatic progress in the strength to density ratio of materials, that resulted in a wide variety of new products, from dental materials to tennis racquets.

![Graph showing the improvement in strength to density ratio over time with labels such as wood, stone, bronze, cast iron, steel, composites, aramid fibers, and carbon fibers.]

**Figure from:** M. A. White, Properties of Materials (Oxford University Press, 1999)
Material science is the investigation of the relationship among processing, structure, properties, and performance of materials.
Structure

• **Subatomic level (Chapter 2)**
  Electronic structure of individual atoms that defines interaction among atoms (interatomic bonding).

• **Atomic level (Chapters 2 & 3)**
  Arrangement of atoms in materials (for the same atoms can have different properties, e.g. two forms of carbon: graphite and diamond)

• **Microscopic structure (Ch. 4)**
  Arrangement of small grains of material that can be identified by microscopy.

• **Macroscopic structure**
  Structural elements that may be viewed with the naked eye.
Length-scales

**Angstrom** = 1Å = 1/10,000,000,000 meter = 10^{-10} m

**Nanometer** = 10 nm = 1/1,000,000,000 meter = 10^{-9} m

**Micrometer** = 1µm = 1/1,000,000 meter = 10^{-6} m

**Millimeter** = 1mm = 1/1,000 meter = 10^{-3} m

Interatomic distance ~ a few Å

A human hair is ~ 50 µm

Elongated bumps that make up the data track on a CD are ~ 0.5 µm wide, minimum 0.83 µm long, and 125 nm high
The Scale of Things (DOE)

**Things Natural**
- Cat: ~0.3 m
- Monarch butterfly: ~0.1 m
- Bee: ~15 mm
- Dust mite: 300 μm
- Human hair: ~50 μm wide
- Fly ash: ~10-20 μm
- Magnetic domains garnet film: 11 μm wide stripes
- Schematic, central core: 10 nm
- DNA: ~2 nm wide
- Atoms of silicon: spacing ~tenths of nm

**Things Manmade**
- Head of a pin: 1-2 mm
- MEMS (MicroElectroMechanical Systems) Devices: 10-100 μm wide
- Red blood cells: ~2-5 μm
- Objects fashioned from metals, ceramics, glasses, polymers...
- Indium arsenide quantum dot
- Quantum dot array – germanium dots on silicon
- Corral diameter 14 nm
- Self-assembled “mushroom”
- Quantum corral of 48 iron atoms on copper surface positioned one at a time with an STM tip
- Coral diameter 14 nm

Progress in atomic-level understanding

**Chart from http://www.sc.doe.gov/production/bes/scale_of_things.html**
Length and Time Scales in Materials Modeling

by Greg Odegard, NASA
Length and Time Scales in Materials Modeling

Mesoscopic

- Dislocation Dynamics

Mo Li, JHU, Atomistic model of a nanocrystalline

Microscopic

- Farid Abraham, IBM
  - MD of crack propagation

Leonid Zhigilei, UVA
- Phase transformation on diamond surfaces

Nanoscopic

- Elizabeth Holm, Sandia
  - Intergranular fracture
  - Monte Carlo Potts model

0.1

1

$10^{-9}$ $10^{-7}$ $10^{-5}$ $10^{3}$ $10^{5}$ $10^{7}$ $10^{9}$ $10^{11}$

Length Scale, meters

Length Scale, number of atoms

Time Scale, seconds
Types of Materials

Let us classify materials according to the way the atoms are bound together (Chapter 2).

**Metals:** valence electrons are detached from atoms, and spread in an 'electron sea' that "glues" the ions together. Strong, ductile, conduct electricity and heat well, are shiny if polished.

**Semiconductors:** the bonding is covalent (electrons are shared between atoms). Their electrical properties depend strongly on minute proportions of contaminants. Examples: Si, Ge, GaAs.

**Ceramics:** atoms behave like either positive or negative ions, and are bound by Coulomb forces. They are usually combinations of metals or semiconductors with oxygen, nitrogen or carbon (oxides, nitrides, and carbides). Hard, brittle, insulators. Examples: glass, porcelain.

**Polymers:** are bound by covalent forces and also by weak van der Waals forces, and usually based on C and H. They decompose at moderate temperatures (100 – 400 C), and are lightweight. Examples: plastics rubber.
Properties

Properties are the way the material responds to the environment and external forces.

**Mechanical** properties – response to mechanical forces, strength, etc.

**Electrical** and **magnetic** properties - response electrical and magnetic fields, conductivity, etc.

**Thermal** properties are related to transmission of heat and heat capacity.

**Optical** properties include to absorption, transmission and scattering of light.

**Chemical stability** in contact with the environment - corrosion resistance.
Material Selection

Different materials exhibit different crystal structures (Chapter 3) and resultant properties.
Material Selection

Different materials exhibit different microstructures (Chapter 4) and resultant properties.

Superplastic deformation involves low-stress sliding along grain boundaries, a complex process of which material scientists have limited knowledge and that is a subject of current investigations.
Material selection: Properties/performance and cost

<table>
<thead>
<tr>
<th></th>
<th>Strength</th>
<th>Ductility</th>
<th>Cost</th>
<th>Final selection</th>
</tr>
</thead>
<tbody>
<tr>
<td>Metals</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ceramics</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Polymers</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Semiconductors</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Composites</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

metals

semiconductors

ceramics

polymers
Composition, Bonding, Crystal Structure and Microstructure DEFINE Materials Properties

Composition

Bonding ↔ Crystal Structure

Thermomechanical Processing

Microstructure
Future of materials science

Design of materials having specific desired characteristics directly from our knowledge of atomic structure.

• **Miniaturization:** “Nanostructured" materials, with microstructure that has length scales between 1 and 100 nanometers with unusual properties. Electronic components, materials for quantum computing.

• **Smart materials:** airplane wings that adjust to the air flow conditions, buildings that stabilize themselves in earthquakes…

• **Environment-friendly materials:** biodegradable or photodegradable plastics, advances in nuclear waste processing, etc.

• **Learning from Nature:** shells and biological hard tissue can be as strong as the most advanced laboratory-produced ceramics, mollusces produce biocompatible adhesives that we do not know how to reproduce…

• Materials for lightweight batteries with high storage densities, for turbine blades that can operate at 2500°C, room-temperature superconductors? chemical sensors (artificial nose) of extremely high sensitivity, cotton shirts that never require ironing…