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

Europe

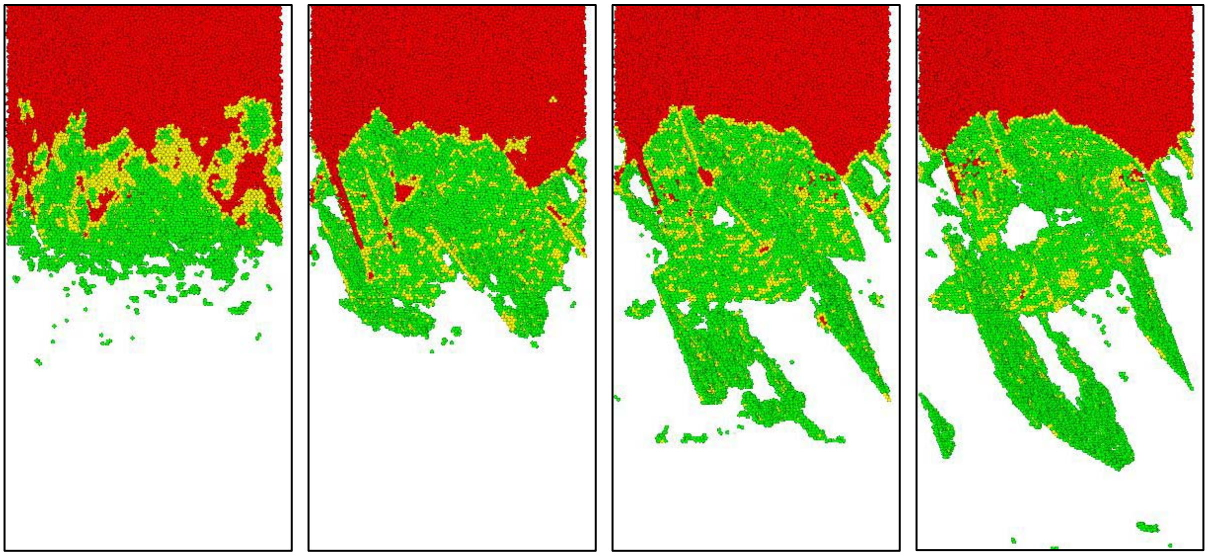
Serbia and Montenegro have asserted the formation of a joint independent state, but this entity has not been formally recognized as a state by the United States.

Macedonia has proclaimed independent statehood but has not been formally recognized as a state by the United States.

Scale 1:19,500,000
Lambert Conformal Conic Projection,
standard parallels 40°N 56°N

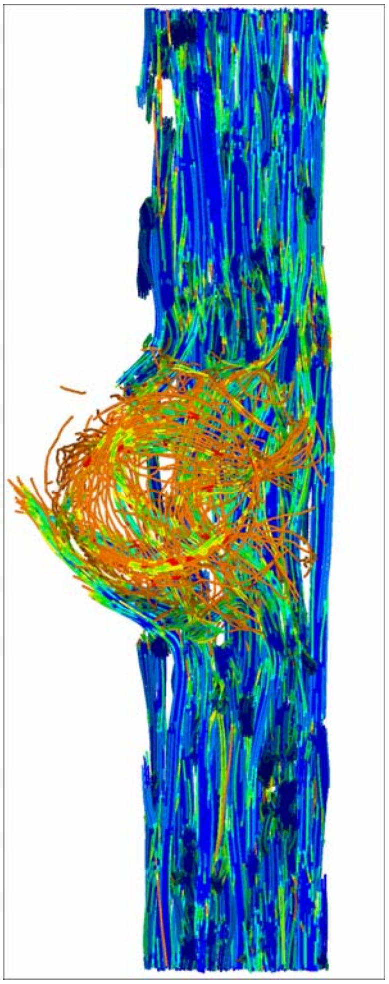
802176 (R01083) 9-93

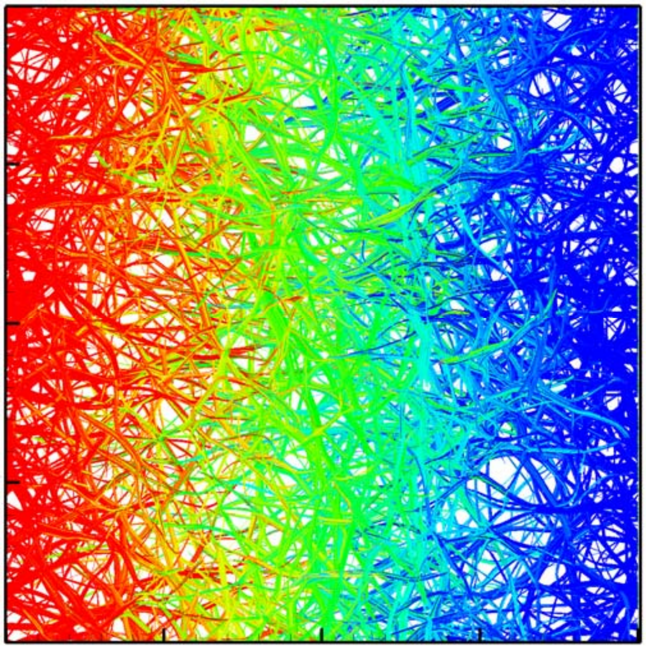
Research in Computational Materials Group:



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:

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Office Hours: 10:00 am to 12:00 pm Tuesday *& open*

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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 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:

W. D. Callister & D. G. Rethwisch, Materials Science and Engineering: An Introduction (John Wiley 2010, 8th edition)

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.

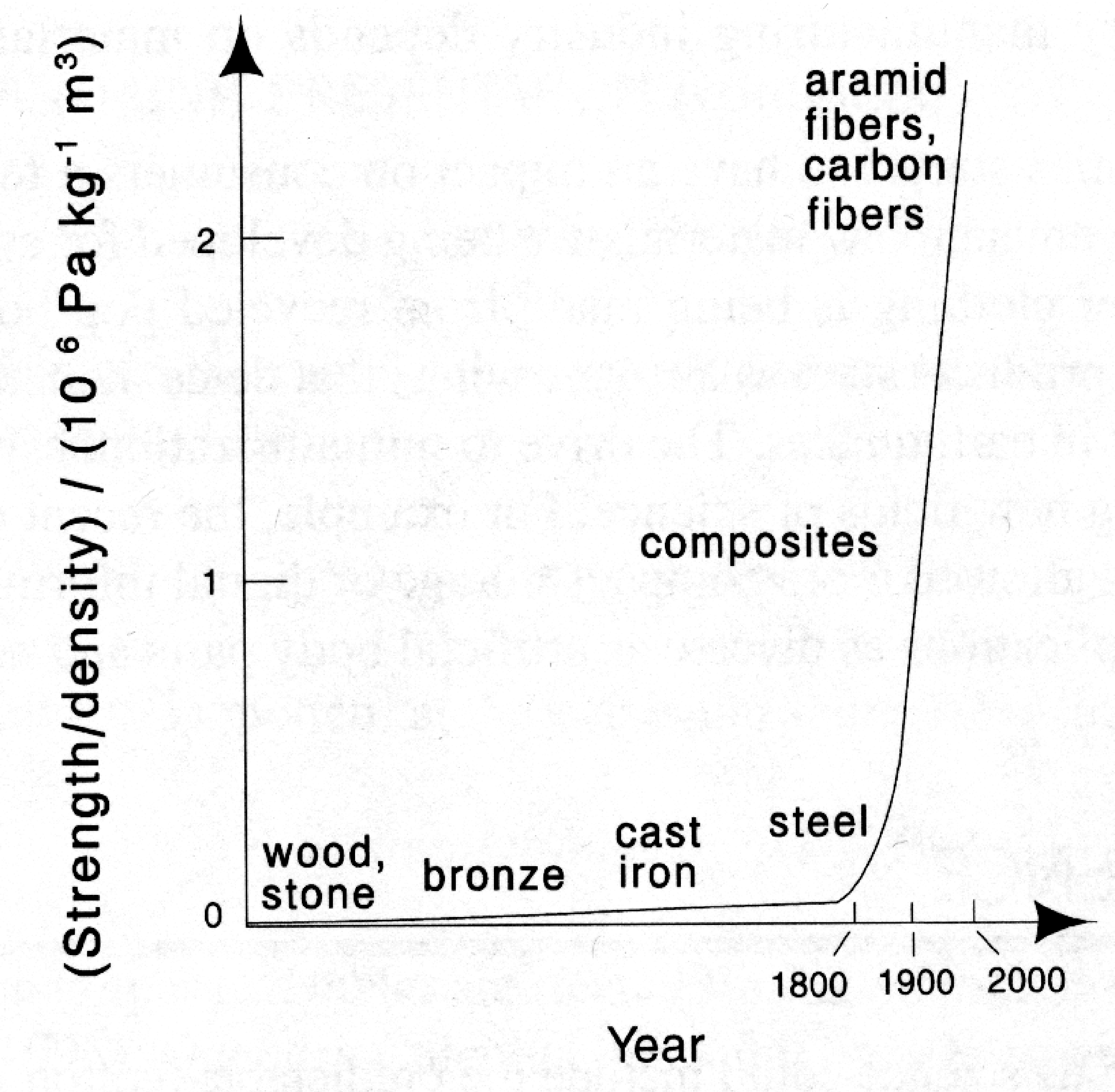
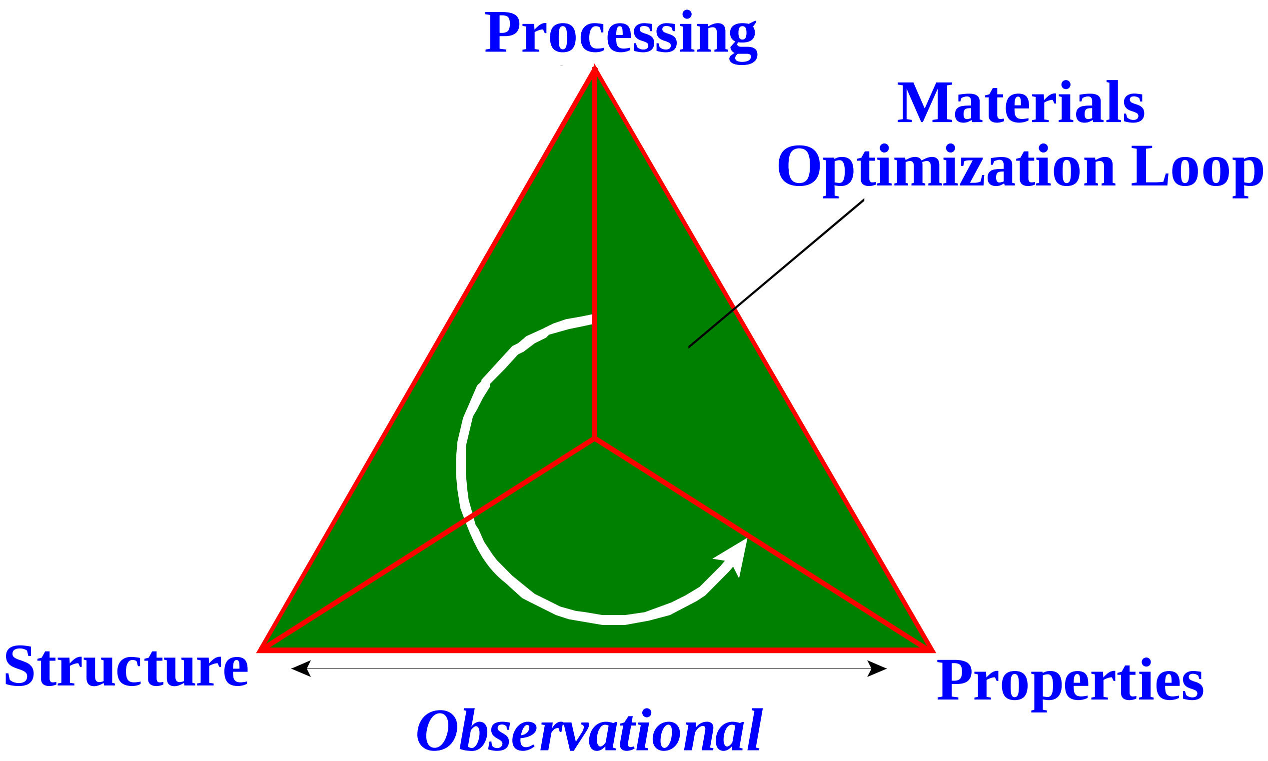


Figure from: M. A. White, Properties of Materials (Oxford University Press, 1999)

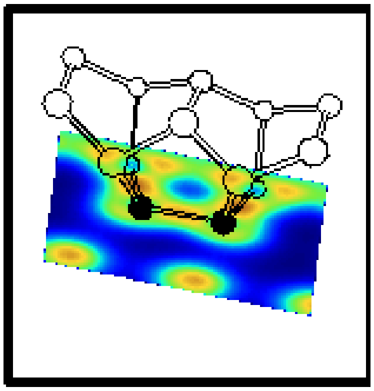
What is Materials Science and Engineering ?



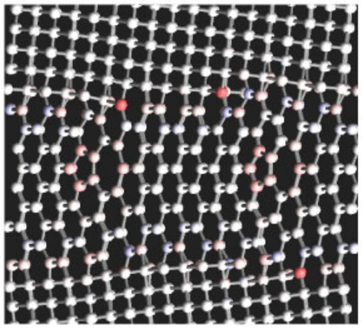
Material science is the investigation of the relationship among processing, structure, properties, and performance of materials.

Structure

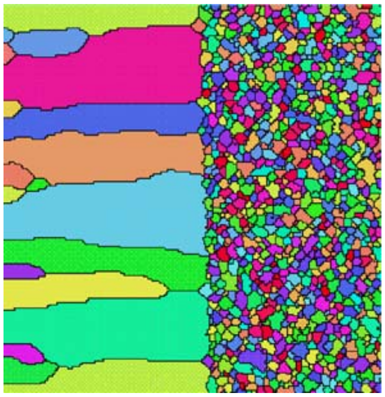
- **Subatomic level (Chapter 2)**
  Electronic structure of individual atoms that defines interaction among atoms (interatomic bonding).



- **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

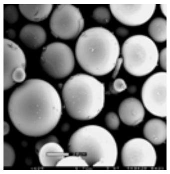

Cat
~ 0.3 m


Monarch butterfly
~ 0.1 m

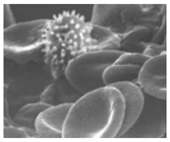

Dust mite
300 µm


Human hair
~ 50 µm wide


Bee
~ 15 mm


Fly ash
~ 10-20 µm

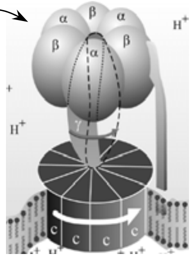

Magnetic domains
garnet film
11 µm wide stripes


Red blood cells
with white cell
~ 2-5 µm

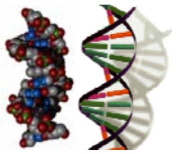
Schematic, central core

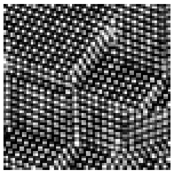

10 nm

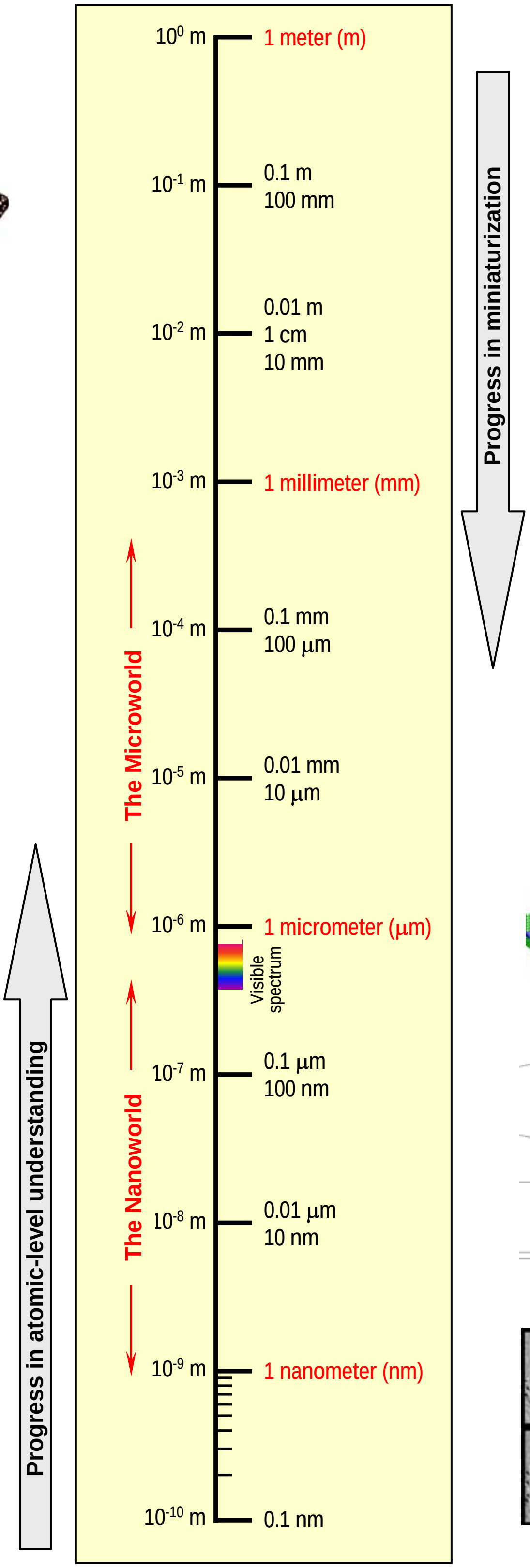
ATP synthase



Cell membrane


DNA
~2 nm wide

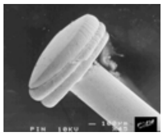

Atoms of silicon
spacing ~tenths of nm

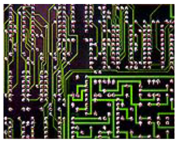


Things Manmade

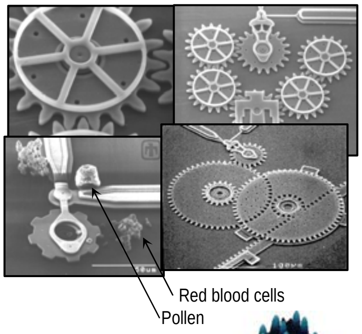

Objects fashioned from
metals, ceramics, glasses, polymers ...

Head of a pin
1-2 mm

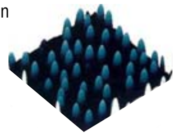


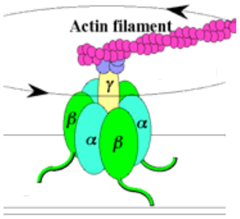

Microelectronics

MEMS (MicroElectroMechanical Systems) Devices
10 -100 µm wide

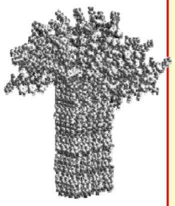


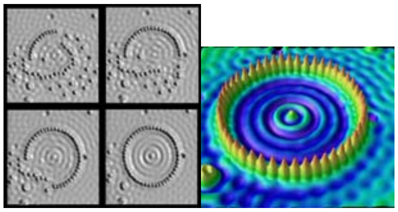

Indium arsenide
quantum dot

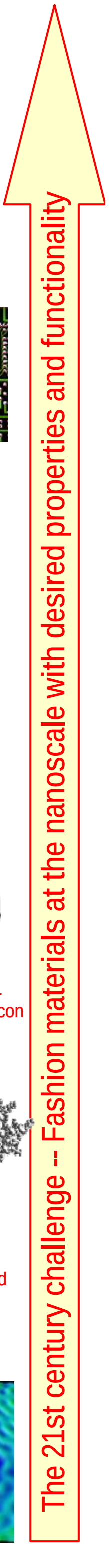

Quantum dot array --
germanium dots on silicon



Biomotor using ATP


Self-assembled
"mushroom"


Quantum corral of 48 iron atoms on copper surface
positioned one at a time with an STM tip
Corral diameter 14 nm

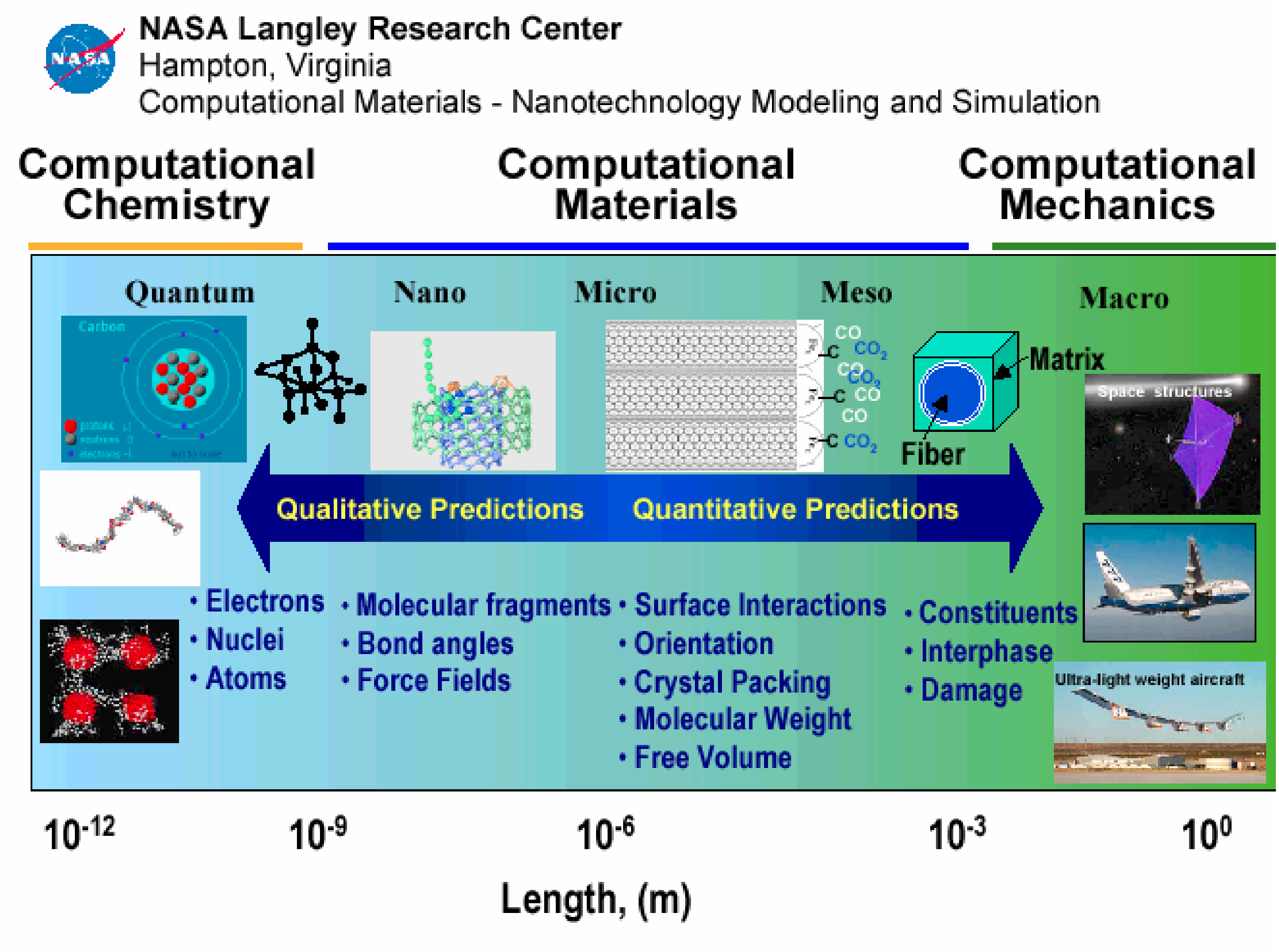


meter	m	10^{0}	1 m
centimeter	cm	10^{-2}	0.01 m
millimeter	mm	10^{-3}	0.001 m
micrometer	µm	10^{-6}	0.000001 m
nanometer	nm	10^{-9}	0.000000001 m

Chart from http://www.sc.doe.gov/production/bes/scale_of_things.html

Length and Time Scales in Materials Modeling

by Greg Odegard, NASA



NASA Langley Research Center
Hampton, Virginia
Computational Materials - Nanotechnology Modeling and Simulation

Computational Chemistry | **Computational Materials** | **Computational Mechanics**

Quantum | Nano | Micro | Meso | Macro

Qualitative Predictions ↔ Quantitative Predictions

- Electrons
- Nuclei
- Atoms

- Molecular fragments
- Bond angles
- Force Fields

- Surface Interactions
- Orientation
- Crystal Packing
- Molecular Weight
- Free Volume

- Constituents
- Interphase
- Damage

10^{-12} 10^{-9} 10^{-6} 10^{-3} 10^{0}

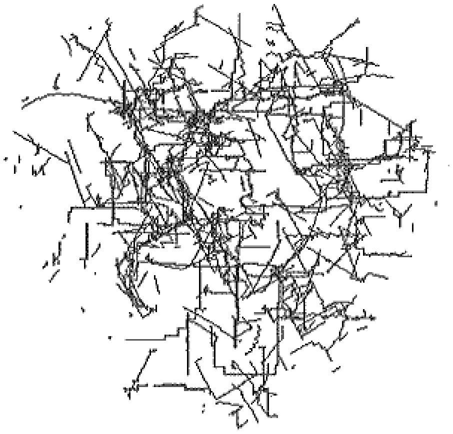
Length, (m)

Length and Time Scales in Materials Modeling

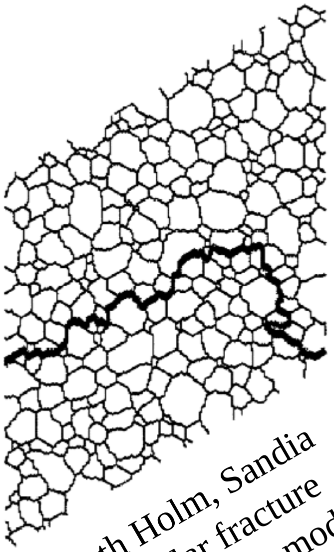
10^{-9} → 10^{-8} → 10^{-7} → Length Scale, meters → 0.1 →

10^{3} → 10^{6} → 10^{9} → Length Scale, number of atoms → 10^{27} →

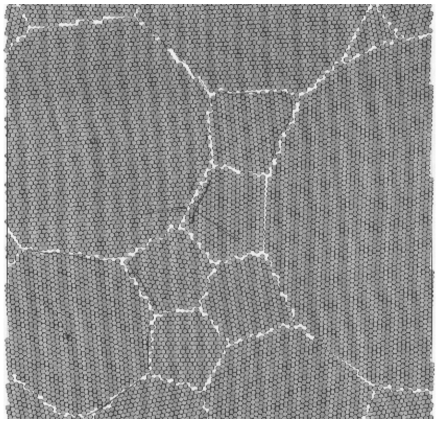
Mesoscopic



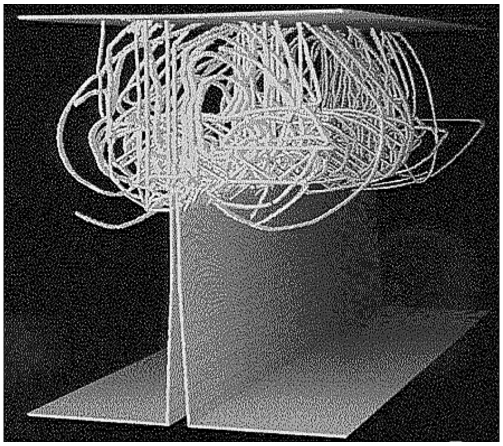
Dislocation Dynamics
Nature, 12 February, 1998



Elizabeth Holm, Sandia
Intergranular fracture
Monte Carlo Potts model



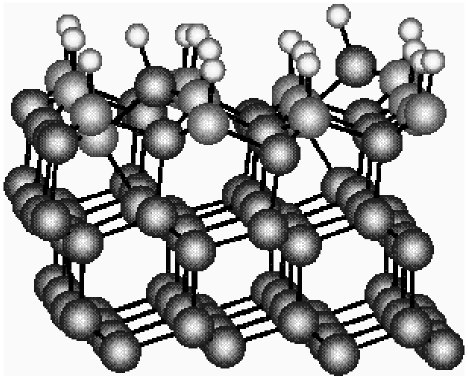
Mo Li, JHU, Atomistic
model of a nanocrystalline



Farid Abraham, IBM
MD of crack propagation

Microscopic

Nanoscopic



Leonid Zhigilei, UVA
Phase transformation on
diamond surfaces

10^{-12} → 10^{-9} → 10^{-7} → Time Scale, seconds → 1 →

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.

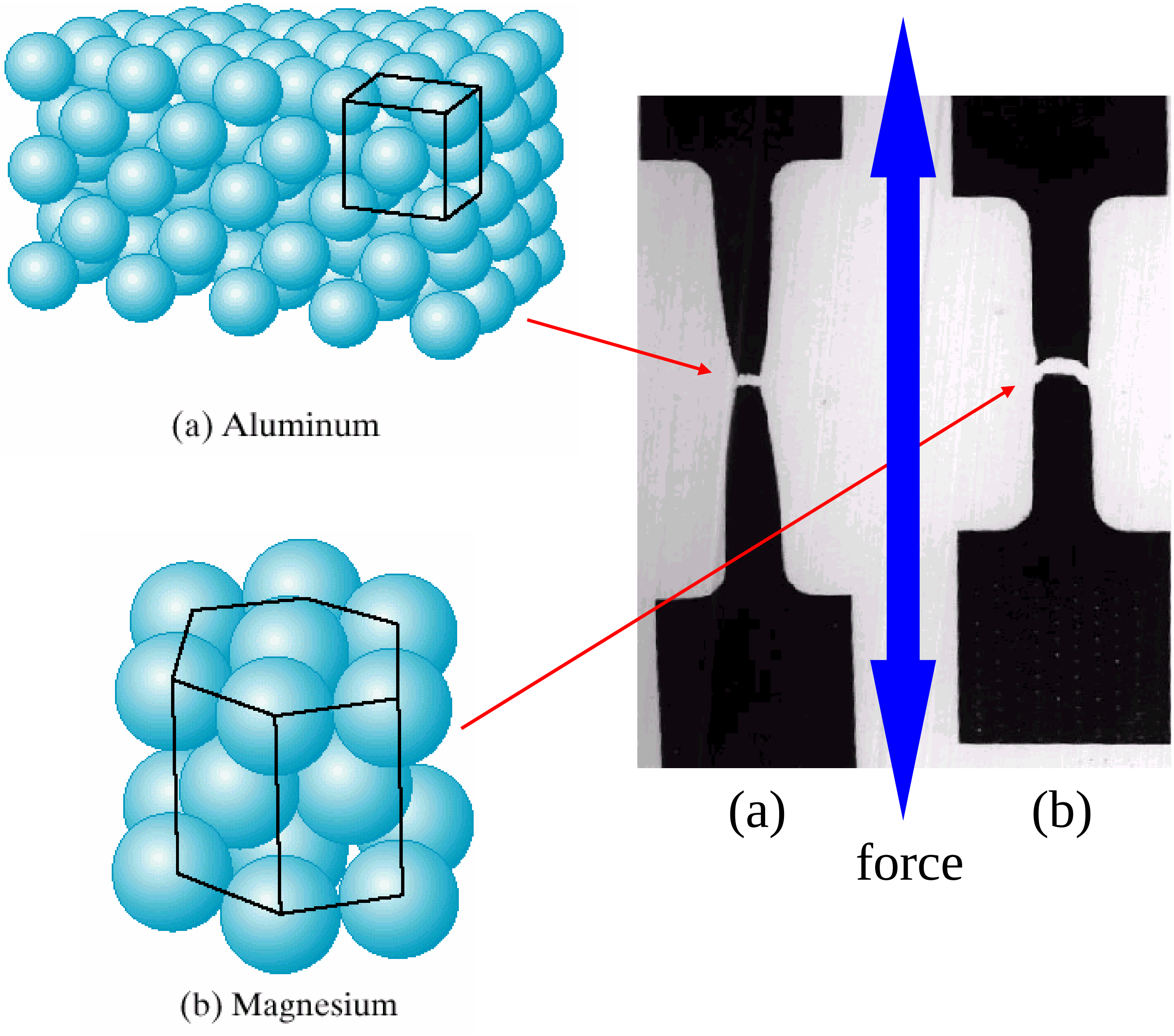
Thermal properties are related to transmission of heat and heat capacity.

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

Chemical stability in contact with the environment - corrosion resistance.

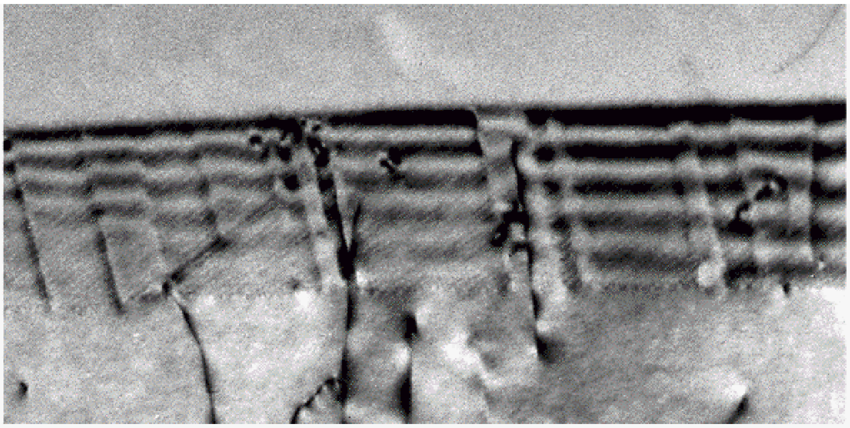
Material Selection

Different materials exhibit different **crystal structures** (Chapter 3) and resultant **properties**

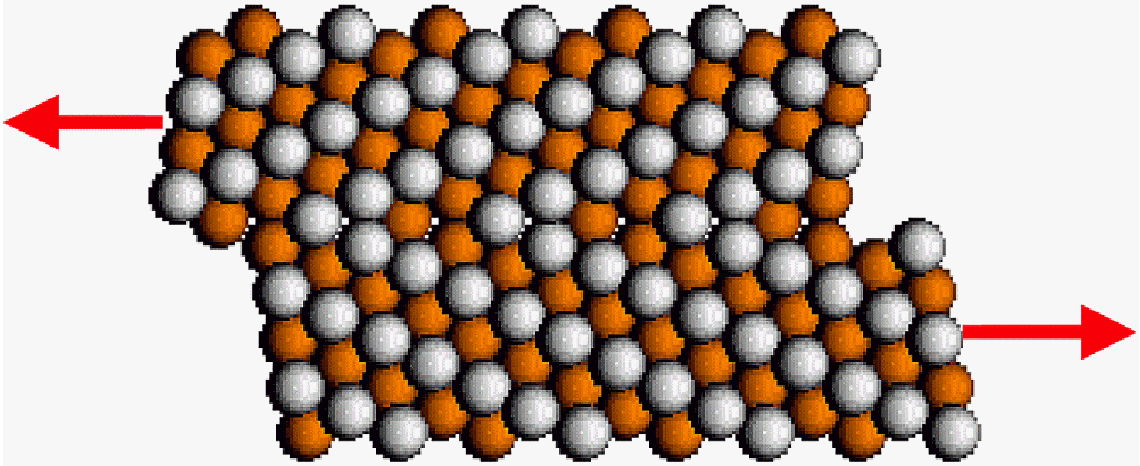


Material Selection

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



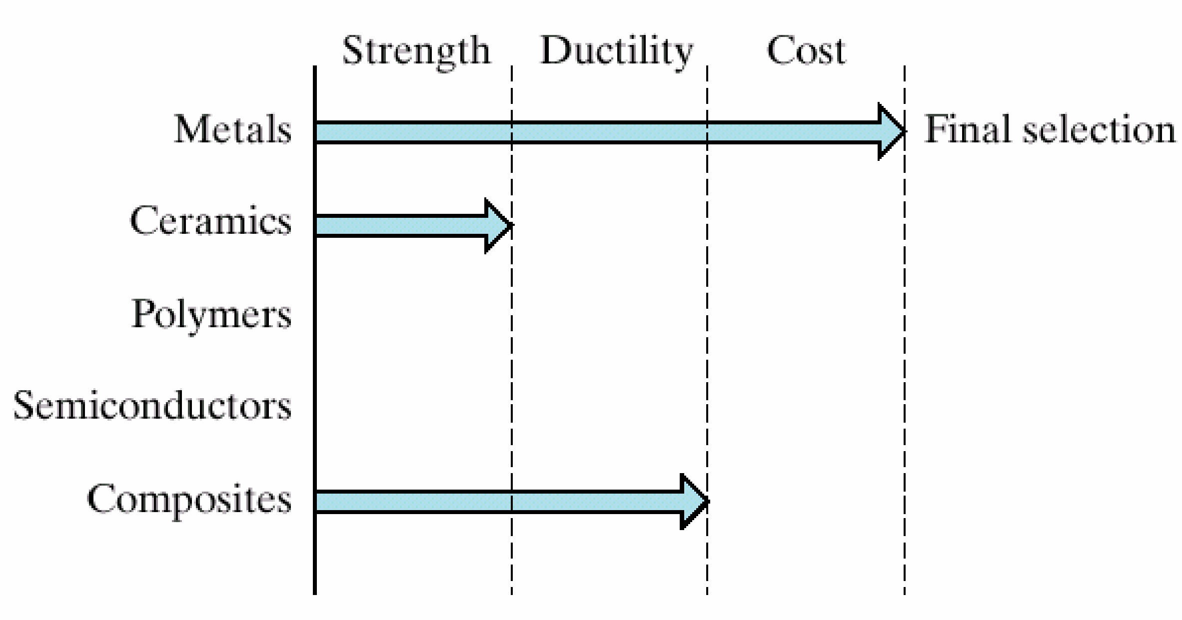
Extrinsic grain boundary dislocations in Al

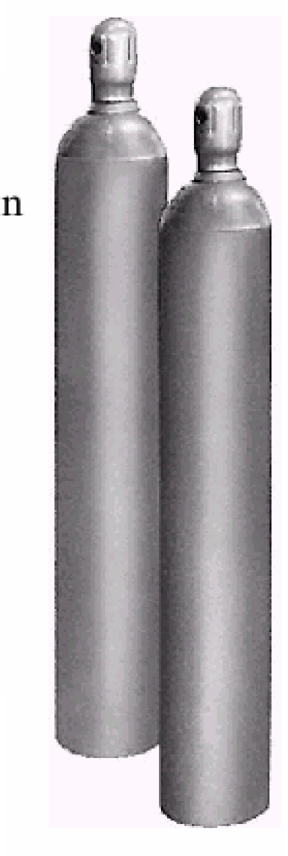


Sliding of defect free Σ11 {131} grain boundary

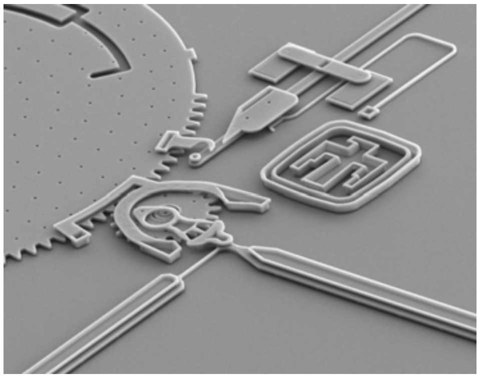
Superplastic deformation involves low-stress sliding along grain boundaries, a complex process of which material scientists have limited knowledge and that is a subject of current investigations.

Material selection: Properties/performance and cost

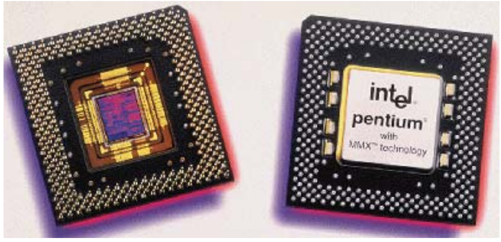


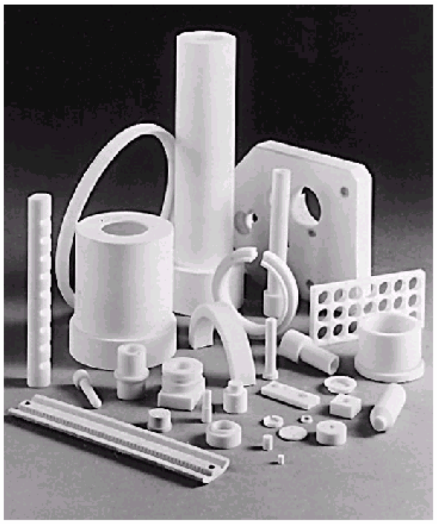


metals



semiconductors

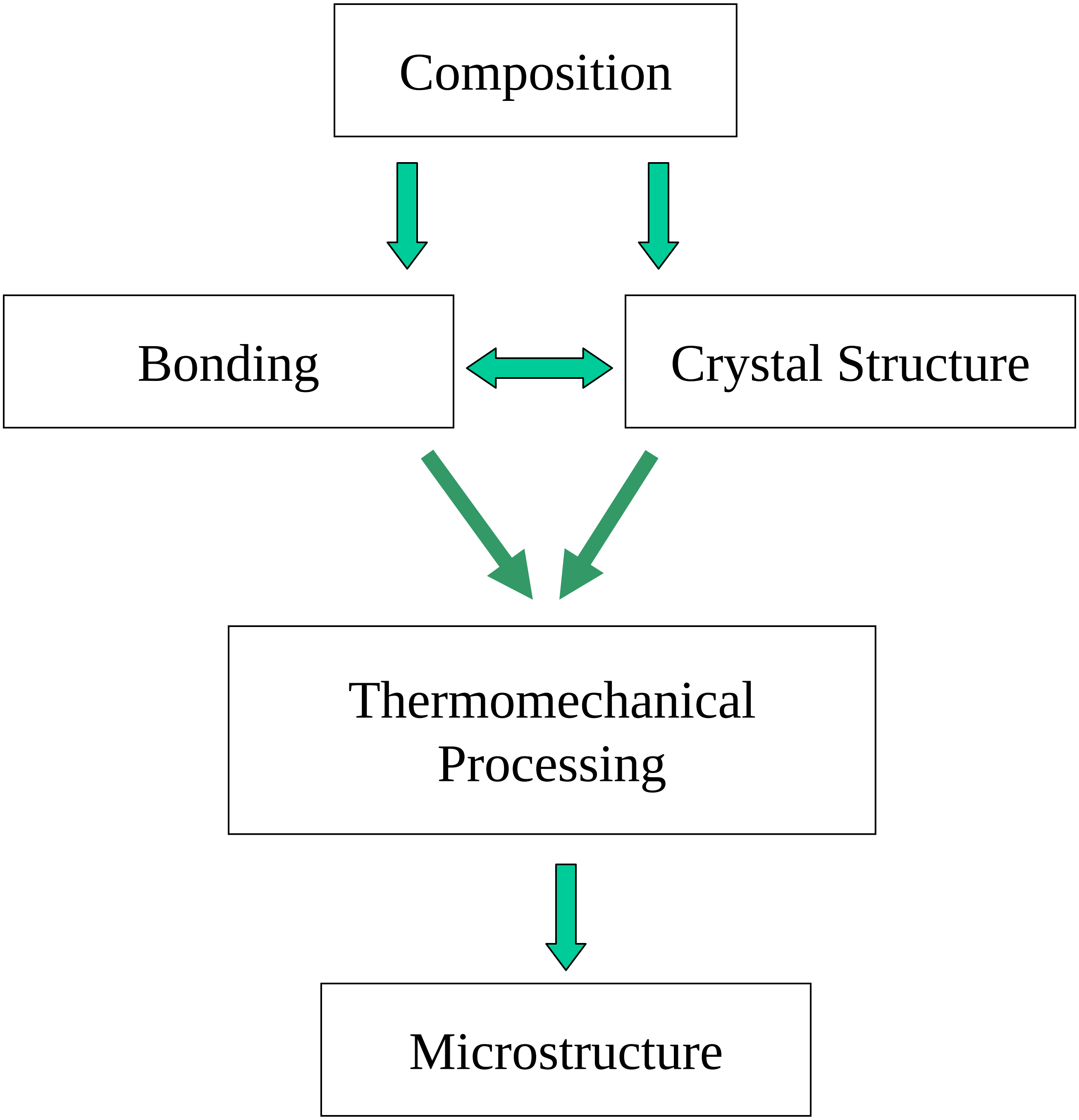




ceramics

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…