

Survey of Materials. Lecture 1

Basics of Materials Science

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Outline

- Understanding scales
- Classification of materials
- Bonding in molecules and solids

MSE tetrahedron & scales: Mechanical properties

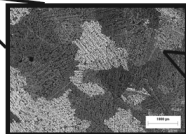
What is Materials Science and Engineering?



Macro-Scale Structure
Engine Block
≅ upto 1 meter

Performance Criteria

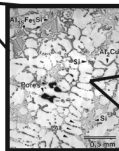
- Power generated
- Efficiency
- Durability
- Cost



Microstructure
- Grains
≅ 1 – 10 millimeters

Properties affected

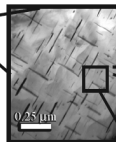
- High cycle fatigue
- Ductility



Microstructure
- Dendrites & Phases
≅ 50 – 500 micrometers

Properties affected

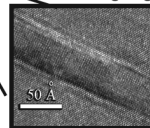
- Yield strength
- Ultimate tensile strength
- High cycle fatigue
- Low cycle fatigue
- Thermal Growth
- Ductility



Nano-structure
- Precipitates
≅ 3-100 nanometers

Properties affected

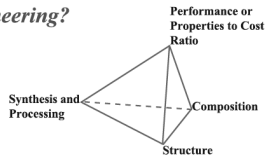
- Yield strength
- Ultimate tensile strength
- Low cycle fatigue
- Ductility



Atomic-scale structure
≅ 1-100 Angstroms

Properties affected

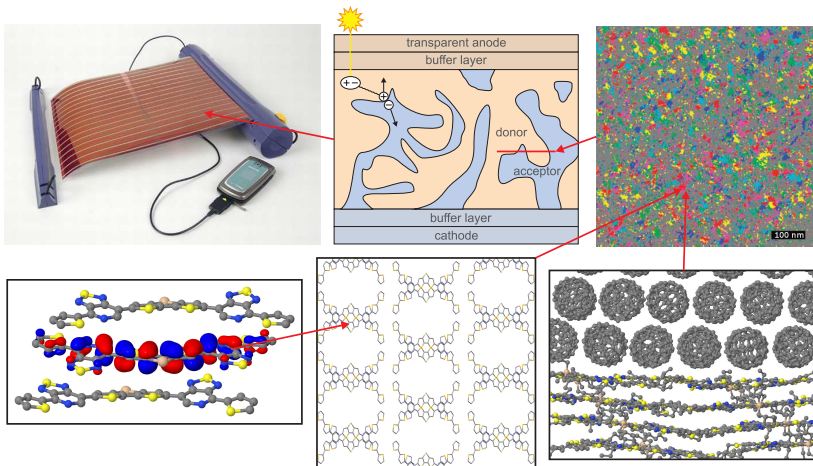
- Young's modulus
- Thermal Growth



A real-world example of important microstructural features at different length-scales, resulting from the sophisticated synthesis and processing used, and the properties they influence. The atomic, nano, micro, and macro-scale structures of cast aluminum alloys (for engine blocks) in relation to the properties affected and performance are shown. The materials science and engineering (MSE) tetrahedron that represents this approach is shown in the upper right corner.

(Illustrations Courtesy of John Allison and William Donlon, Ford Motor Company)

MSE tetrahedron & scales: Electronic properties



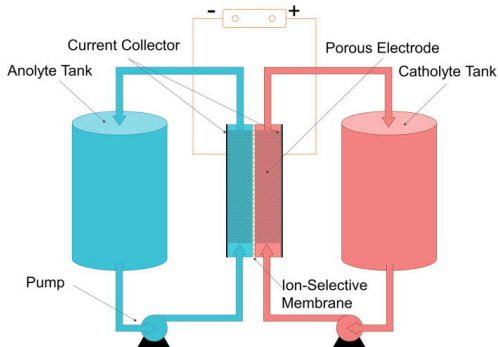
Synthesis &
Processing

– **Structure – Properties** –

Engineering &
Technology

Understanding scales: 'off the shelf' example

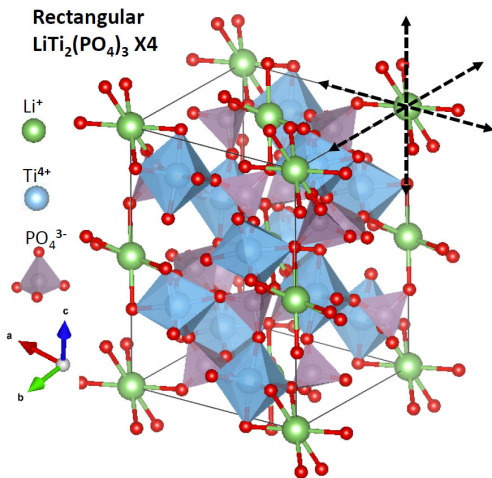
Ongoing project: developing membrane for redox flow battery



Key properties to optimize:

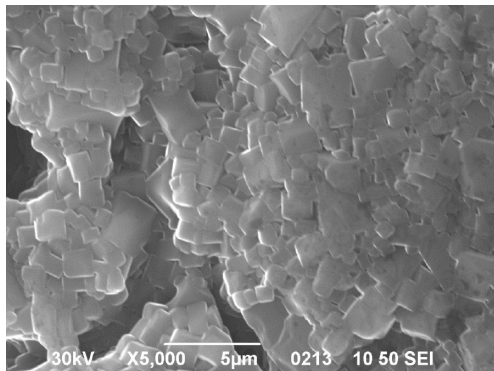
- High ionic conductivity and low electronic conductivity
- Selectivity
- Chemical and mechanical stability

Atomistic scale: optimize chemical composition



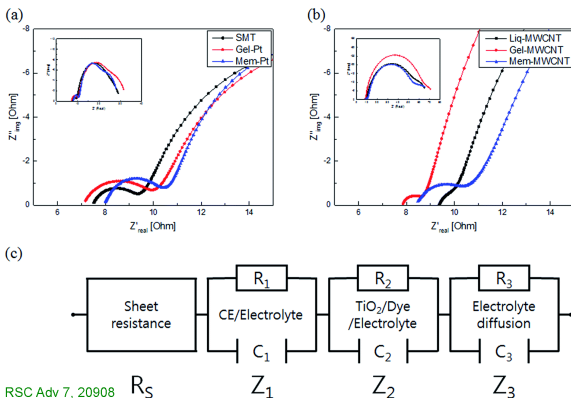
Single-material scale: optimize synthesis and morphology

(solid state synthesis, X-ray, TEM)

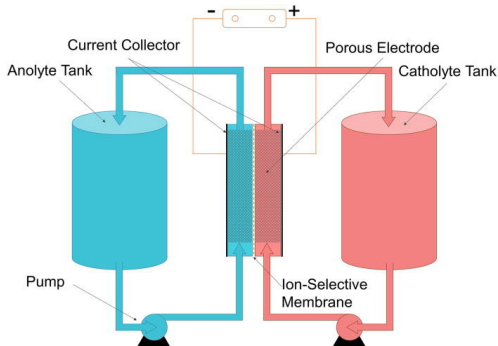


Device scale: test and optimize device architecture

(electrochemical impedance spectroscopy, aging tests, device modeling and engineering)



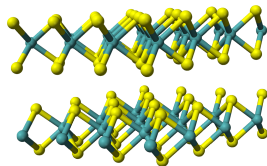
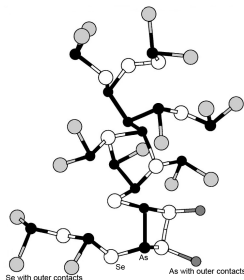
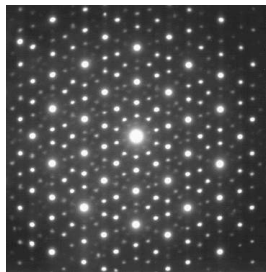
Real membrane in redox flow battery



- High ionic conductivity and low electronic conductivity
- Selectivity
- Chemical and mechanical stability

Now you can patent it, then consider other parts, upscale and commercialize

Classification by structure



- crystals, polycrystals, quasicrystals, liquid vs plastic crystals
- liquids, glasses, amorphous solids, (gases)
- surfaces and low-dimensional materials, polymers
- mixtures and nanostructured materials: solutions, blends, composites, interfaces, sandwich structures, adsorbates, thin films ...

Classification by properties

- **mechanical properties:** metals, plastics, ceramics, composites, fibers, glasses
- **electronic structure:** metals, semimetals, semiconductors, insulators, superconductors, graphene, topological insulators
- **electrical conductivity:** metals, semiconductors, insulators, superconductors, solid ionic conductors, electrolytes
- **electric properties:** dielectrics, high- k dielectrics, piezoelectrics, pyroelectrics, ferroelectrics, capacitors
- **optical properties:** light absorbers, conducting transparent oxides, chiral crystals, nonlinear optical materials
- **magnetic properties:** ferromagnetics, magneto-optical materials
- **nanoporous materials:** zeolites, clathrates

Classification by processing technology

- **metallurgy**: metals and alloys
- **3D printing**: plastics, metals, ceramics; rapid prototyping, additive manufacturing
- **semiconductor fabrication plants (fab)**: “2D printing”; classical semiconductors
- **solution processable**: molecules, polymers, ionic solids; spin coating, inkjet printing; R2R processing, printed electronics
- **chemical vapor deposition (CVD)**: highest quality solids
- **graphene and 2D**: special processing
- **biosynthesis/biodegradation**: biomolecules and biopolymers; low-cost, low-energy, environment-friendly

Bonding in molecules and solids

Given a chemical composition:

- Predict structural preferences
- Estimate binding (cohesion) energy: $E(A) + E(B) - E(AB)$
- Speculate on functional properties

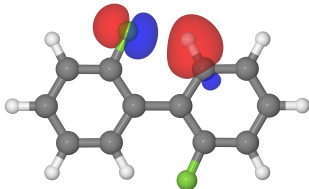
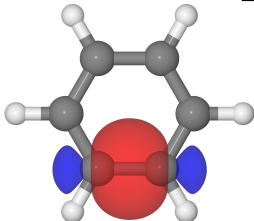
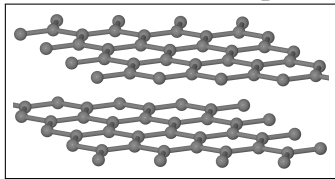
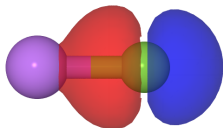
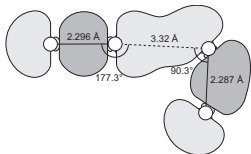
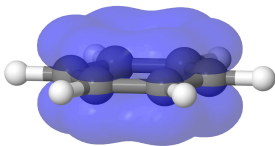
Sets of simple rules and concepts:

- **Atomic radii** (metallic, covalent, ionic, vdW)
- Close packing for isotropic interactions
- **Valence shell electron pair repulsion (VSEPR) theory** for molecules and covalent solids
- **Huckel's rule** for π -conjugated molecules
- **Hume-Rothery rules** for alloys
- ...

Accurate empirical potentials (force fields, EAM, EIM, COMB)

Bonding: Basic interactions

- covalent
 - ionic
 - metallic
-
- steric
 - donor-acceptor
 - residual chemical
-
- hydrogen
-
- electrostatic
 - London dispersion
 - medium mediated
 - other physical



H_2O vs SO_2 vs CH_4

Summary and Resources

See summary [here](#)

- Wikipedia
- [Crystal structures](#)
- [Crystallography Open Database](#)
- References: [structure](#), [bonding](#)
- [Textbooks](#)