Research Area = Materials Physics/Condensed matter physics

Methods = Experiment coupled with theory/computation

Research Goals
- New Materials Discovery
- Physics of materials
- Superior Properties

Mechanical, Thermoelectronic, Magnetic properties
Some of the Tools

- X-ray diffraction
- Atomic force microscopy
- Low energy electron microscope
- Materials synthesis
- Electrical transport measurement
- Magnetic measurement
- Ultrasound measurement

Graphs and images showing various measurements and materials synthesis techniques.
Physics of States of Matter
Amorphous/Glassy Metals
Glasses are ubiquitous in nature, e.g. optoelectronic, window, copy machine, biological systems.

Glasses are highly frustrated systems with strong particle-particle correlations.

Glassy state can be described by multi-dimensional energy landscape, and shares much of the physics of spin glass, neural network and protein folding.

More ……

Why some systems are trapped in the glassy state? What are the properties? How to improve glass formability?
**Superior Properties**

High strength per unit mass, Soft magnetism, Superior surface properties

**Application Areas**
- Transportation systems
- Space vehicle/structure
- Micro-machines/actuators/sensors
- Transformers
- Electric engines
- Surface coating
- Catalysis

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![Stress (GPa) vs Elastic Strain (%) diagram]

- Ceramic
- Steel
- Ti
- Glassy metals
- Polymeric
- Amorphous Steel discovered @ UVa
Physics of Glassy Metals

Multi-component systems
→ Complexity science
Atomistic scale design
Atomistic scale structure

**Density Functional Theory (DFT)**

\[
E_{xc}[\rho(x)] = T_{\rho}[\rho(x)] + E_{el}[\rho(x)] + E_{xc}[\rho(x)] + E_{ext}[\rho(x)]
\]

\[
\rho(x) = \sum_n a_n |\phi_n(x)|^2
\]

\[
\{-\frac{\nabla^2}{2m} + V_{\text{eff}}(x) - \varepsilon_n\} \phi_n(x) = 0
\]

\[
V_{\text{eff}}(x) = V_{\text{ext}}(x) + \Phi(\rho(x)) + \mu_{xc}(\rho(x))
\]

**Molecular Dynamics (MD)**

\[
F_i(\varepsilon) = -\frac{\partial V(r_1(\varepsilon), r_2(\varepsilon), \ldots, r_N(\varepsilon))}{\partial r_i(\varepsilon)}
\]

\[
v_i(\varepsilon + \Delta\varepsilon) = v_i(\varepsilon - \Delta\varepsilon/2) + F_i(\varepsilon) \Delta t
\]

\[
r_i(\varepsilon + \Delta\varepsilon) - r_i(\varepsilon) + v_i(\varepsilon + \Delta\varepsilon/2)\Delta t
\]
Harvesting Energy through Thermoelectrics: Power Generation and Cooling

(clockwise from left) Figure of merit ZT shown as a function of temperature for several bulk thermoelectric materials; schematic representation of a power-generating thermoelectric module; photograph of a radioisotope thermoelectric generator (courtesy of NASA/JPL-Caltech); and the crystal structure of CoSb$_3$ (skutterudite) with "rattler" atoms (in red). In the background is a photograph of the Voyager spacecraft, which was fitted with a radioisotope thermoelectric generator (courtesy of NASA/JPL-Caltech). See the technical theme that begins on p. 188.
Skutterudites

Half-Heuslers

ZrCoSb

LaCo₄Sb₁₂

Clathrates

Ba₈Ga₁₆Ge₃₀

Chevrel Phases

La₂Te₃

Cu₄Mo₆Se₈

Th₃P₄
Metallic crystals exhibit unusual electronic structure

Example of unusual electronic structures – interplay of orbitals and crystal structure
Scientific issues of interest

- Bandgap material - interesting thermoelectronic properties
- Magnetic state with gapless spin-up band and gapped spin-down band (spin-polarized state)
Thermoelectric materials are used in electronic refrigeration and power generation. The materials are environmentally “green”.

The devices are compact and involve no moving parts.

Cooling of computer chips (CPU), low noise amplifiers, IR detectors…

Power generation using waste heat - Space (NASA) and Naval applications.
Radioisotope TE Generator (RTG) 250W

Fission reactor Power (100 kW)
High Temperature: 1000 C hot, 500 C cold
TE or Brayton Engine for energy conversion

- Weight, Size, Reliability are issues
- shielding, heat rejection panels,
  ion propulsion, science package, $B

Missions
Jupiter Icy Moons Orbiter
Mars/Lunar Missions

• Pu\textsuperscript{238}O\textsubscript{2} Heat Source
  - “Safe” - α decay
    88 year half life
• Voyager & Pioneer > 25 years
  - SiGe TE elements
  - 250 W for 50 kg
    Necessary for outer planet missions
    low solar flux, (Cassini, Galileo)
• Next Generation (MMRTG)
  - PbTe/TAGS TE elements
**Thermoelectric Performance** is defined by a dimensionless figure-of-merit = $ZT$, $Z = \frac{S^2}{\rho \kappa}$ or $\frac{S^2 \sigma}{\kappa}$, where $S$ = Seebeck thermopower, $\rho$ = resistivity, $\kappa$ = thermal conductivity.

State-of-the-art $ZT \approx 1$

$ZT >> 1$ needed to $\rightarrow$ Carnot efficiency

$ZT \sim 2-3$ great!
- New electronic materials can lead to high $S^2\sigma$.

- Atomic- and nano-scale structural design can lead to low $\kappa$. 

**ZT of our new compounds matches SiGe**
Why study Nanostructured and Glassy Solids?

1. Can form a broader range of materials
   (non-equilibrium methods involve short length and time scales)
   resulting in new magnetic, structural, thermoelectronic materials

2. Investigate non-crystalline properties

3. Investigate size dependence of properties

Nanocrystalline State
Crystal size confines electronic and vibrational states, modifies spectra, dislocation structure and scattering.
Magnetic Behavior of Nanostructure

- Microstructural features smaller than domain wall width
- No domain wall pinning on nanocrystals
Nanostructured Magnetic Materials

Electric Power Systems
- High density power
- High speed machines
- Materials breakthroughs

- Spin manipulation
- Transformer cores
- Hard disk drive
- Cassette recording heads
- Ultrahigh density media