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Materials Science and Technology Team Introduction

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Materials Science

- New materials have tremendous impact in energy, information technology, health, transportation, and other applications.

- **Energy:** high temperature applications, solar photovoltaics, and light emission.
- **Information technology:** Materials integration and processing with nanometer precision.
- **Structural materials:** longer fatigue lives, higher strengths, and better wear characteristics

- **New concepts:** theory, synthesis, and characterization: crystal growth, processing far from equilibrium, nanopatterning, and hierarchical self-assembly

Materials Science and Technology Team

- Members:
  - Paul Evans (Wisconsin) chair
  - Kathy Faber (NWU)
  - John Mitchell (Argonne)
  - Cev Noyan (Columbia)
  - Carol Thompson (NIU)
  - Choong-Shik Yoo (Washington State)
- Email: mst.renewal@mailman.aps.anl.gov

Goals and Draft Report

- Goals: Identify several exciting specific opportunities within the very broad context of materials science.
- Draft report available at:

  http://www.aps.anl.gov/Renewal/Reports/materials_science.pdf

Length and Timescales

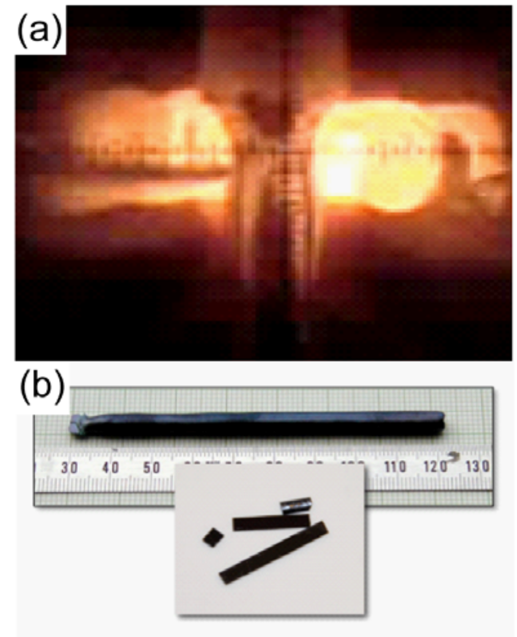
- ***Small length scales*** from the positions of single atoms to the overall organization of materials at large scales.
- ***Dynamic processes*** The properties and structure of materials evolve during these times, leading to the need for a fundamentally new approach to *in situ* studies.
- ***Random untriggerable events***

Key Areas of Scientific Opportunities

1. **Crystal growth:** What phases and processes are relevant to the growth of bulk crystals?
2. **Dynamic compression:** What are the properties of materials under transient pressures far higher than those available in static experiments?
3. **Imaging random events:** How can we understand the rare stochastic events behind nucleation and crack initiation and other seemingly random incidents?
4. **Atomic positions in semiconductor devices, ultimate strain:** What are the positions of atoms in devices with sizes on the order of tens of nanometers? How do the concepts of strain, composition, and concentration apply at this scale?
5. **Dynamics in applied fields:** What is the structural response of materials to applied electric and magnetic fields?

1. Bulk Crystal Growth

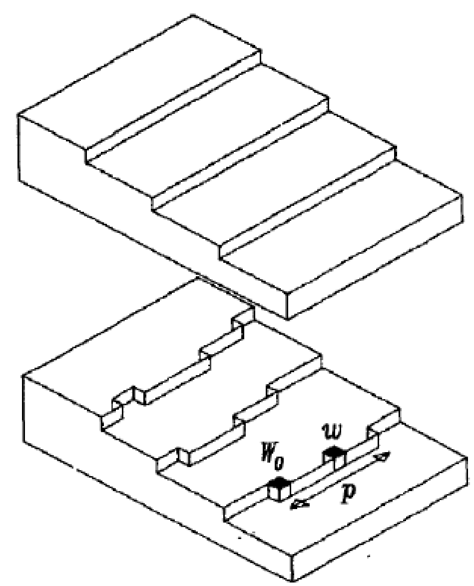
- *Floating-zone growth*
- *High-pressure crystal growth*
- *Hydrothermal synthesis*
- *Flux growth*
- *Biological/Protein Crystal Growth and Self-Assembly*



In comparison with epitaxial growth, bulk crystal growth is still largely an art form.

Crystal Growth

- Bulk crystals of many potentially important materials simply are not available
  - – III-Nitrides (GaN, etc.)
  - – PZT
- What phases are relevant under growth conditions? What atomic processes are involved in crystal growth?



Terrace-step-kink model
(From Robinson and Tweet 1996)

2. Dynamic Compression

- *Extreme conditions:*
  - *In the condensed state pressures are up to 500-1000 GPa (5-10 Mbar) and temperatures to 0.5 eV (5000 K).*
  - *Variation of thermodynamic variables: P, V, T, S over wide range.*
  - *Interplay of $P\Delta V$ and $T\Delta S$.*
  - *Transient conditions: μs or shorter times*

3. Imaging Random Events

- Nucleation, domain wall motion, cracking, nucleation, and other events are essentially random and difficult to trigger.
- New approach: “Time reversal imaging”
  - – Use the high bandwidth and data rate of new detectors to change the way data is taken.
  - – Create structural images and diffraction patterns at a high rate and save them if a random event of interest occurs.

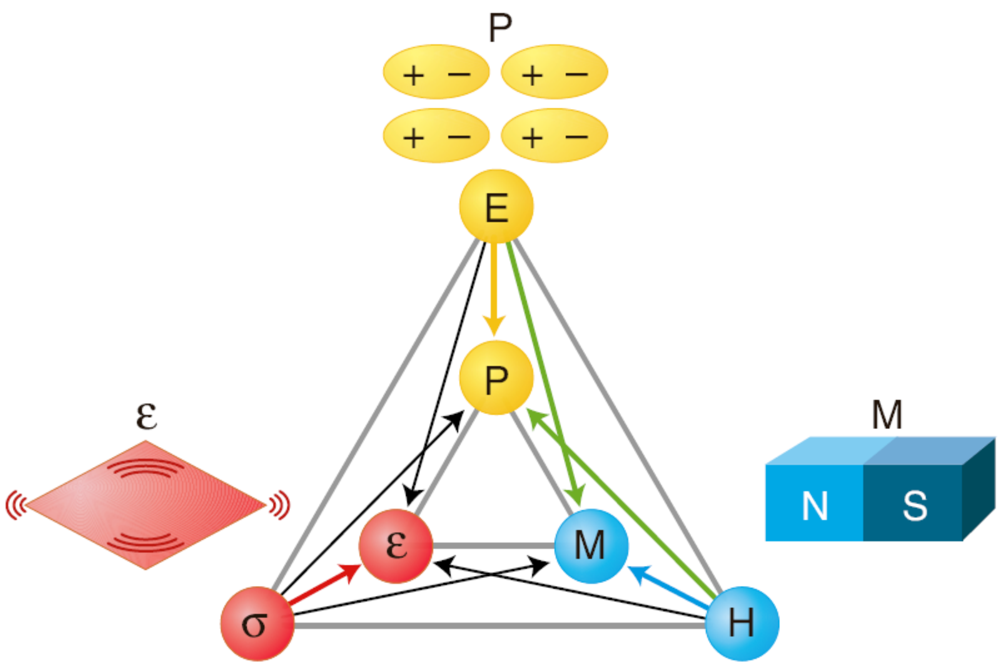
Imaging Random Events

- Crack initiation and growth under monotonic loading in brittle materials.
- Fatigue crack initiation and growth in metals.
- Pitting during aqueous or gas-phase corrosion.
- Environmental-assisted or embrittlement of grain boundaries. These experiments would highlight which grain boundaries are more susceptible to embrittlement than others.
- Vortices in superconductors and other nano-to-mesoscale phenomena in condensed matter systems.

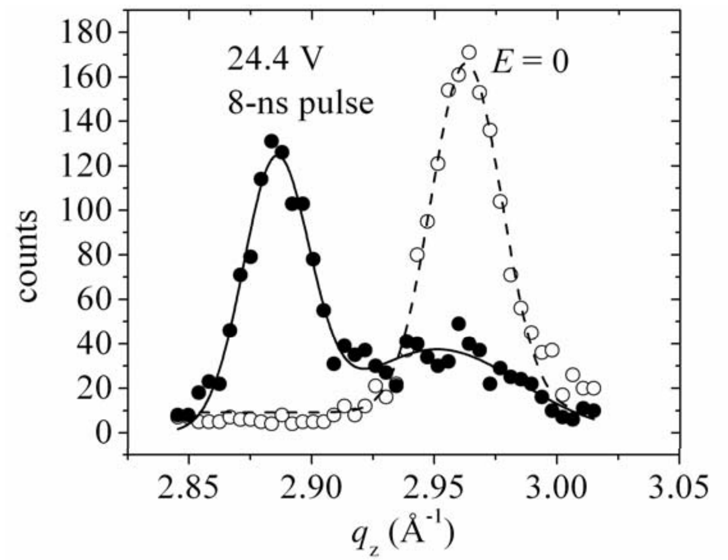
4. Atomic positions in semiconductor devices, ultimate limits of strain

- Semiconductor devices are already 50 nm-scale nanostructure (only 100's of atoms across!)
- No rigorous definition of normalized displacement: strain is difficult to define at scales of 10 nm or less
- Interaction of strain fields between adjacent structures
- How can we meet this characterization challenge?

5. Dynamics in applied fields

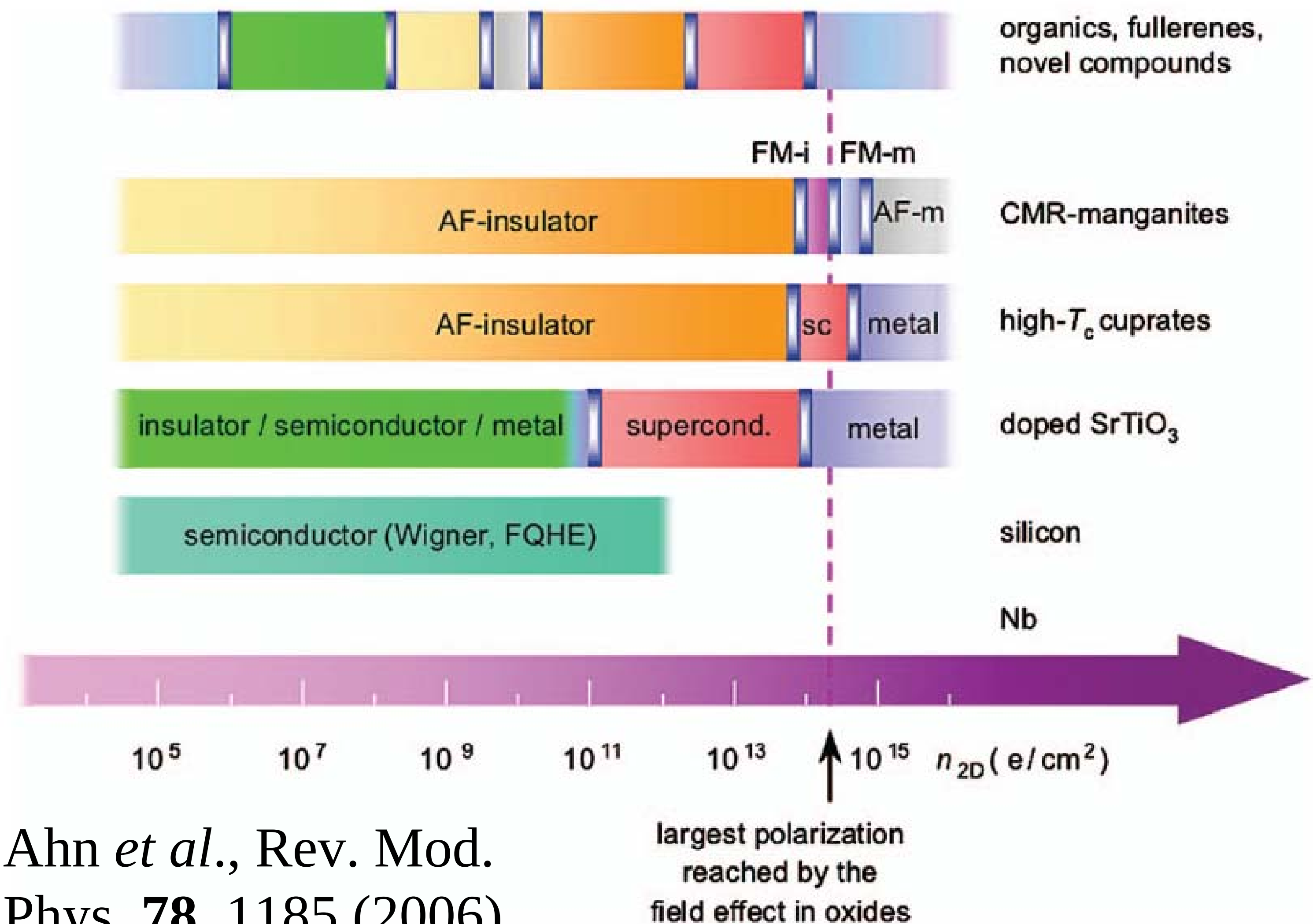


N. A. Spaldin and M. Fiebig, Science **309**, 391 (2005).



Transient strain of 2.7% in a 40 nm-thick PZT film in response to an 8 ns electric field pulse, Grigoryev *et al*. Phys. Rev. Lett. **100**, 027604 (2008).

Applicable to a Wide Range of Systems



Ahn *et al*., Rev. Mod. Phys. **78**, 1185 (2006)

Scientific Requirements

Full-Field Microscopy and Tomography

- *Nanodiffraction*
  - Beam-size around 10 nm or better, with energy resolution below 1 eV over 5-30 keV range
- *Dynamics*
  - ***Short Pulse Sources***
- *Environments*

Facility-wide improvements and Infrastructure

- Software to process the stream of data arising from these scattering and imaging tools.
- Advances in beamline control software are necessary to allow these experiments to take place routinely. This improvement in the information infrastructure will simplify use of the APS and allow its capabilities to reach wider groups of materials researchers.
- Better stability in beamline software and hardware must be achieved to allow experiments with *in situ* components.
  - The accelerator side of the APS has developed metrics for the availability of the beam that the allow progress being made in optimizing the facility to be quantified, and a similar push needs to be made for the beamlines.
- Improved point and area detectors for scattering and fluorescence will be required to allow the diffraction and imaging experiments to proceed.
- Infrastructure additions that enable the safe and usable installation of a variety of sample processing and synthesis environments.
- Access modes permitting long term installation of both complex user-designed environments optimized for a particular material system as well as general environmental chambers. Infrastructure needs include adequate ventilation and exhaust systems, ability for gas and chemical handling, cleaning, and sensing.

Significance of APS

- Among U.S. light sources, only the APS has a **large diameter and high electron energy**.
- Bunch spacing is an excellent **match for the capabilities of new detectors** capable of single-bunch time resolution.
- **Beamline-scale electron optics producing short pulses** (as in the proposed APS-based Short-Pulse X-ray Source, SPX) requires the uniquely long time between bunches of the APS.
- The APS is the **home of emerging technologies**: multilayer Laue lens optics for x-ray focusing, high-resolution primary beam monochromators and analyzers for inelastic scattering, and high-pressure research.

Breakout Session

1 PM Paul Evans, University of Wisconsin
"*Welcome and Review of Materials Sci. and Technology Team Draft Report and Goals*"

Part 1: Materials Opportunities X-ray Microscopy and Imaging

1:05 PM Jorg Maser, Advanced Photon Source
"*High Resolution Diffractive X-ray Optics, A Near-Term Perspective*"

1:30 PM Cevdet Noyan, Columbia University
"*Imaging random events and local strain determination*"

1:55 PM Discussion: Microscopy in Materials Science

2:05 PM Break

Part 2: Dynamical and *in situ* Phenomena

2:20 PM Rafael Jaramillo, University of Chicago
"*Dynamics in Antiferromagnets*"

2:45 PM Carol Thompson, Northern Illinois University
"*Nanoscale Dynamics in Complex Oxides*"

3:10 PM Wilson Chiu, University of Connecticut
"*Non-Destructive 3-D Imaging and Analysis of Solid Oxide Fuel Cells*"

3:35 PM Open Session and Discussion of Materials Science and Technology Report

4:00 PM Return to Joint Summary and Discussion Session