Physical Sciences and Advanced Materials at ORNL

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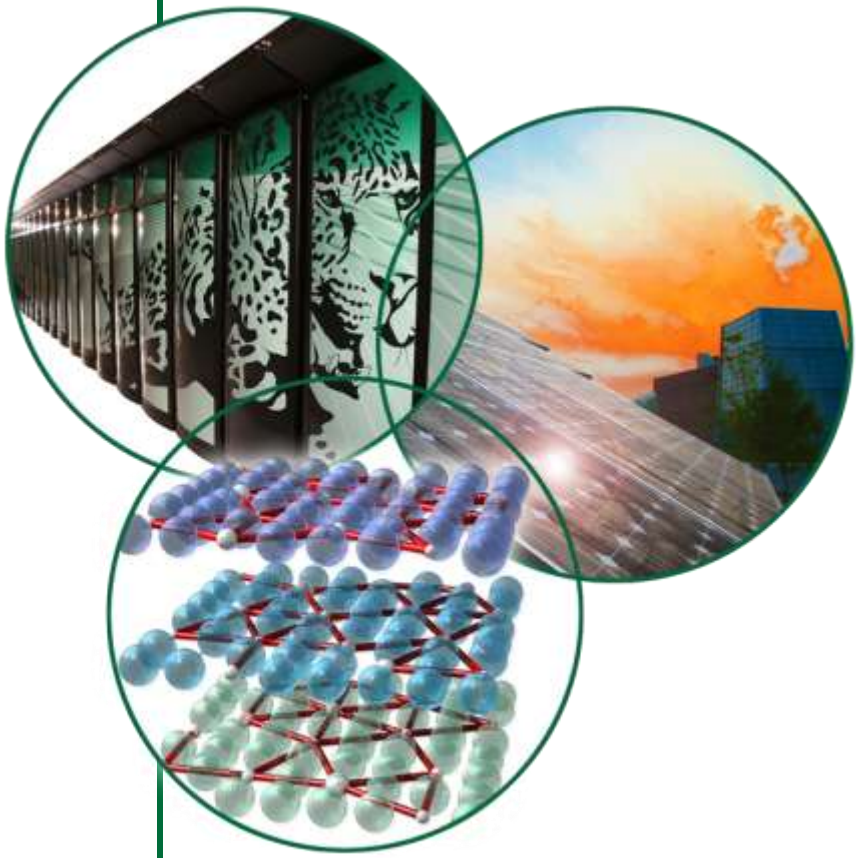
Physical Sciences

September 13, 2010



U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

The Energy Dilemma

- Population growth
- Rampant consumerism
- Emerging economies
- Demand for oil that outstrips supply
- Possible oil supply interruptions
- Increased greenhouse gases

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Today's Energy Resources in U.S.

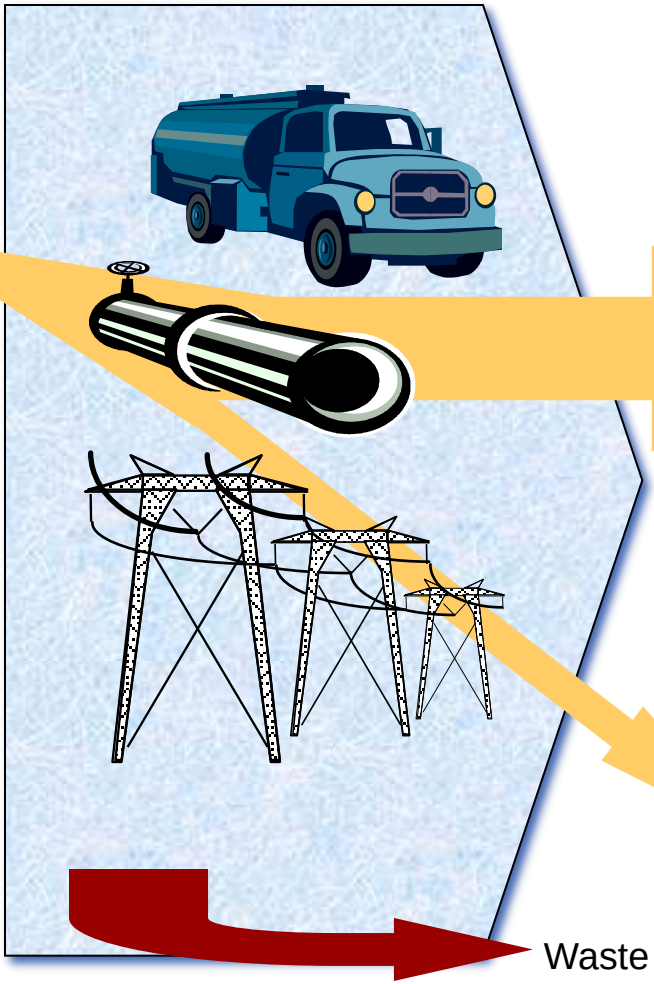
Supply | Distribution | Utilization

100 Quads (3.3 TW)

Fossil
86%

Nuclear
<10%

Renewable
<10%



17% light vehicles
8% freight
3% aircraft

20% homes
commercial

24% industrial

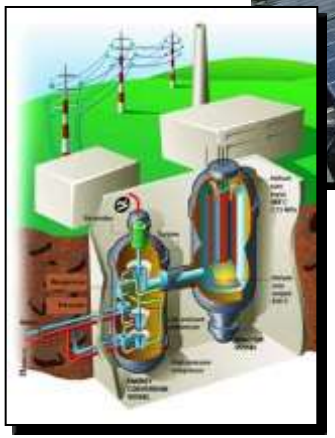
Waste energy 55%

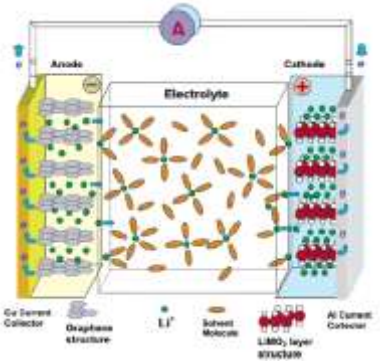
New energy sources and technologies for efficient use are critical for meeting future clean, secure energy requirements

ORNL focus on “Science to Energy”

Advanced materials and interfacial processes for energy

- **Electrical energy storage**
- **Solar**
- **Catalysis**
- **Separations**
- **Nuclear (irradiation, materials, separations)**





Strategy: Take advantage of

- *Unique capabilities in synthesis, characterization, theory*
- *Close coupling of fundamental and applied science*
- *Ties with industry and technology transfer*

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ORNL is unrivaled in advanced materials

DOE's largest materials and condensed matter programs	Special strengths in advanced alloys, correlated electron materials, macromolecular systems, catalysis, synthesis, carbon-based materials, separations
SNS and HFIR offer transforming capabilities	Structure and dynamics, large-scale structures, spins, neutron and neutrino physics
World-class capabilities for nanoscale science	Synthesis, nanoscale characterization, spin-sensitive and other probe spectroscopies
Leadership-class computing	Predictive simulation of materials and molecular interactions
Unmatched characterization capabilities	Electron microscopy, mass spectrometry, local electron probes, physical and chemical properties measurement

DOE's first nanoscience center

World's foremost capabilities for neutron science

Record-setting electron microscopes

Leadership-class computing

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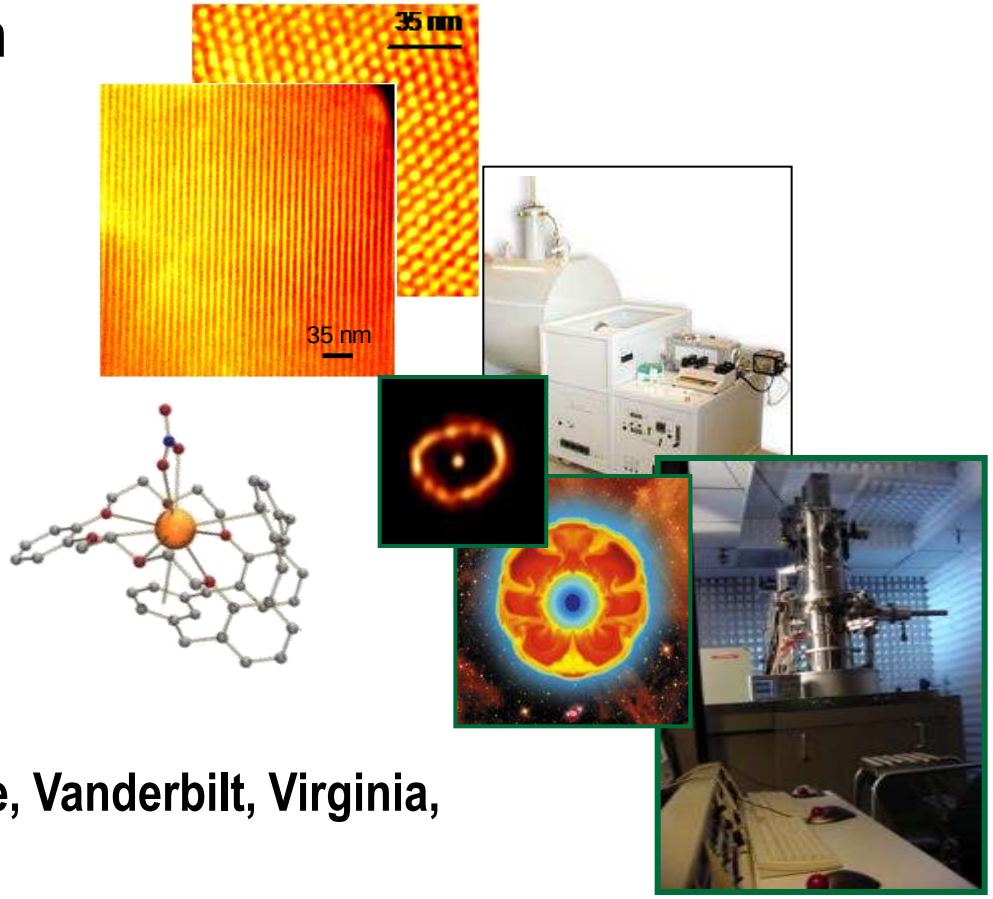
Physical Sciences Directorate

- Home to ORNL core programs in
  - Materials
  - Chemistry
  - Nuclear physics
  - Nanoscience
  - Isotopes
- Approximately
  - ~500 staff
  - >100 post-docs
  - >40 graduate students
  - ~40 joint faculty (including NC State, Vanderbilt, Virginia, Auburn, UT)
- Highly integrated with computational sciences, life sciences, neutron sciences, energy, and national security research programs at ORNL



Leading capabilities

- Condensed matter physics
- Characterization
  - electron microscopy
  - mass spectrometry
  - scanning probes
- Chemical and Materials Theory
- Heavy ion nuclear physics
- Structural materials
- Synthesis
- Materials processing
- Soft materials: polymers and bio
- Separations
- Radiochemical analysis

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ORNL programs in solar PV and electrical energy storage span atomic to system level understanding

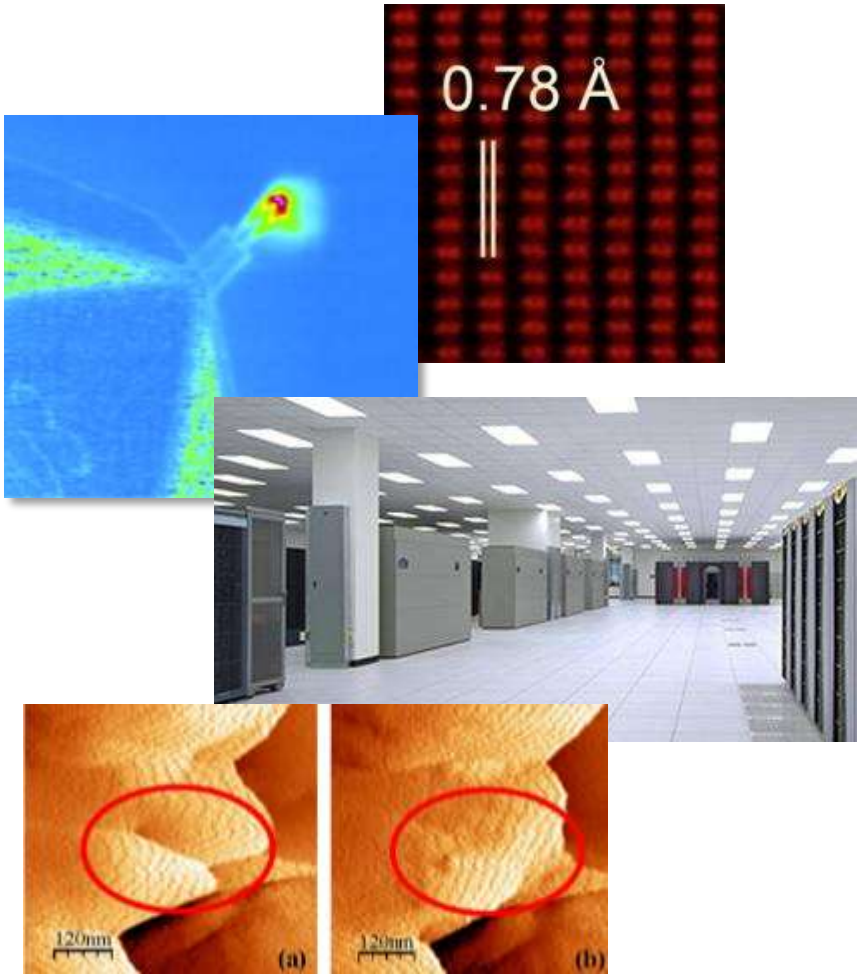
Photovoltaics

- Inorganic PV materials
- Next generation organic PV
- Large scale processing

Electric energy storage

- Novel electrodes
- Ionic liquid, solid, and polymer electrolytes
- Membranes, coatings

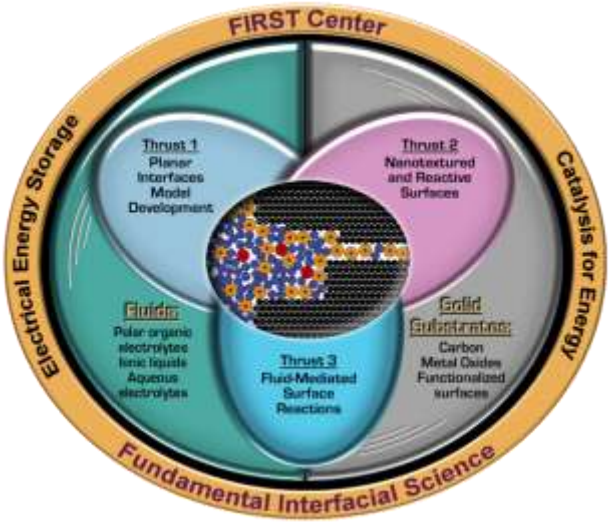
Both areas are supported by state-of-the-art characterization and computational tools



ORNL Awarded Two BES Energy Frontier Research Centers in FY09

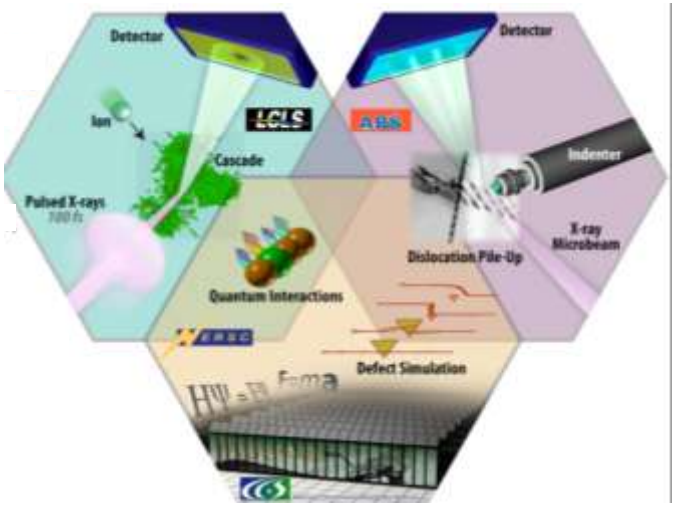
Partners on eight others

Fluid Interface Reactions, Structures and Transport (FIRST)



Study of interfaces in batteries, capacitors, catalysis

Center for Defect Physics in Structural Materials (CDP)



Study of defects in materials under extreme conditions

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Close coupling of science to applications to technology transfer is a key strength of PSD

- PSD has over half of IP at ORNL
  - invention disclosures
  - patents
  - royalties
- Over half of ORNL's IR-100 awards
- Hundreds of industrial collaborators

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Close coupling of science to applications to technology transfer is a key strength of PSD

Applied Materials Portfolio

- EERE (OE, ITP, VT, Solar, etc.)
  - New materials, processing
    - Superconductivity
    - Batteries
    - Solar PV
    - Lightweight materials
      - Carbon composites, new materials
    - Industrial materials
  - HTML User Facility
- Nuclear Energy
  - Comprehensive materials capabilities
  - PIE, new materials, theory
- Fossil Energy
  - New materials, corrosion
- WFO—broad portfolio

control 1.5 x 10^{23} n cm^{-2}

20% CW 316 stainless steel, 796 K

Neutron Damage on SS

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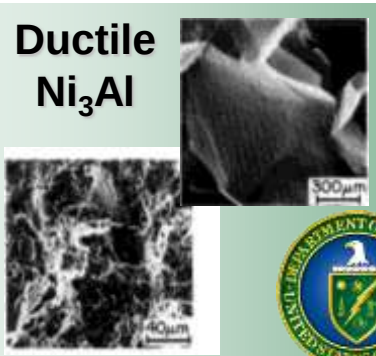
Nickel Aluminides: From Lab Discovery to Commercialization.

Basic Science
(OS, FE)

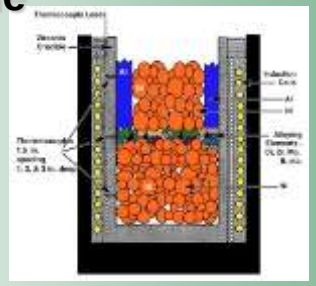
Applied R&D
(EERE Industrial Technologies Program)

Manufacturing & Commercialization

Ductile Ni_3Al



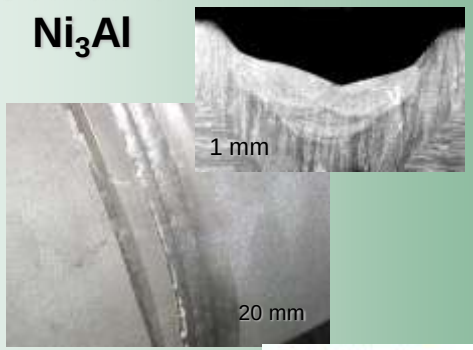
Castable Ni_3Al



✓ Licensed to Duraloy for **fabrication and use of Ni_3Al in Industry for rolls in reheat furnaces.**

Fe-rich nickel aluminide alloy is less expensive & has improved sulfidation resistance:

Joinable Ni_3Al



✓ **Enables 35% increase in furnace energy efficiency.**

✓ **New Ni_3Al melting, casting, and welding materials/processes.**

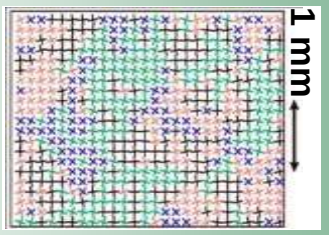
Science to Solutions:
Superconductor Wires: From Lab Discovery to Commercialization

Basic Science
(Office of Science)

Applied R&D
(Office of Electricity Delivery & Energy Reliability)

Manufacturing & Commercialization

Grain-to-grain current flow:



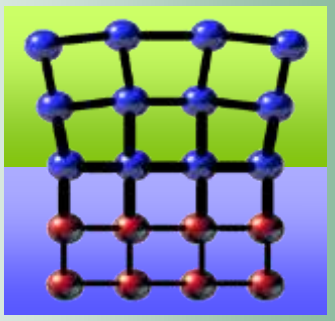
Single crystal-like template by the kilometer (RABiTS™):

- ✓ **Licensed to both major U.S. wire manufacturers.**
- ✓ **Only 2G HTS wire suppliers in the world.**
- ✓ **International customers.**

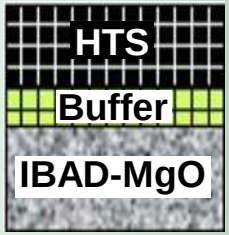
Powered by AMSC

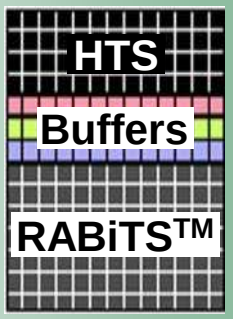
- ***Core template & buffer technologies of AMSC wire.***

Single crystal film formation:



Epitaxial buffers for high-performance 2G HTS wires:





SuperPower Inc.

- ***Key buffer component of SuperPower wire.***

Physical Sciences Divisions operate four DOE user facilities

- Center for Nanophase Materials Science (CNMS)
- High Temperature Materials Laboratory (HTML)
- Holifield Radioactive Ion Beam Facility (HRIBF)
- Shared Research Equipment Program (SHaRE)

Serving > 1000 users / year

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Center for Nanophase Materials Sciences

- Science areas include functional materials, soft materials, catalysis, imaging functionality, bio-nano, theory
- 32 laboratories
- 10,000 sq. ft. clean room
- Nanomaterials Theory Institute
- Office space for 190 staff, visitors, and users
- >$30M in equipment
- Over 400 users in FY09
- Users from universities, industry and national laboratories
- CNMS is recognized for its leadership role in developing ES&H policies for the NanoScience Research Centers

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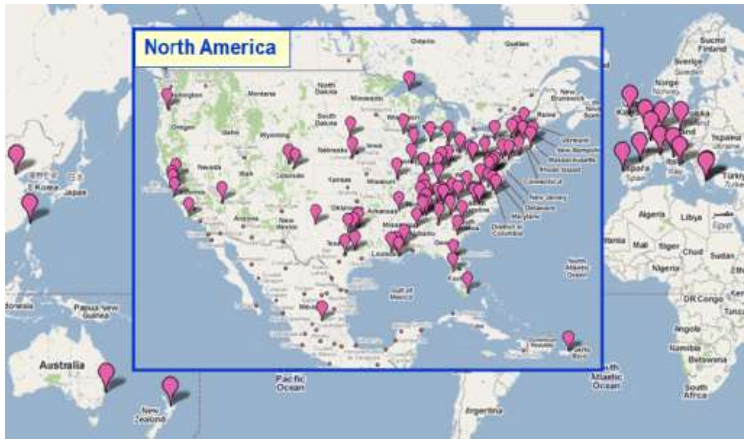
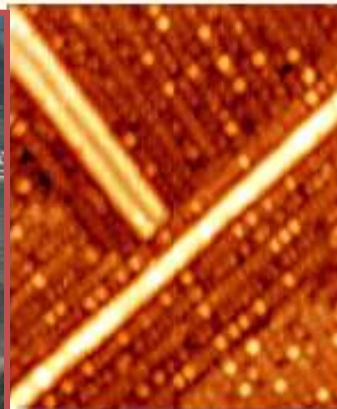
The Center for Nanophase Materials Sciences

Understand, Design, and Control Functionality in Nanoscale Systems:

Key capabilities:

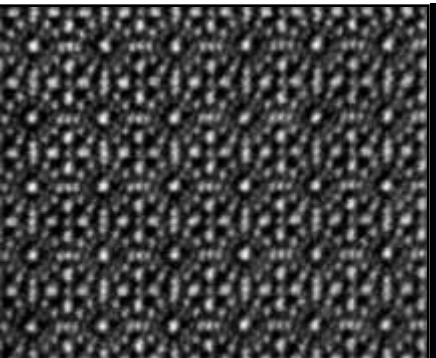
- Polymer synthesis/characterization
- Specialized scanning probes
- Nanomaterials synthesis/ characterization
- Nanofabrication
- Nano Theory Institute
- Close ties to SNS/HFIR

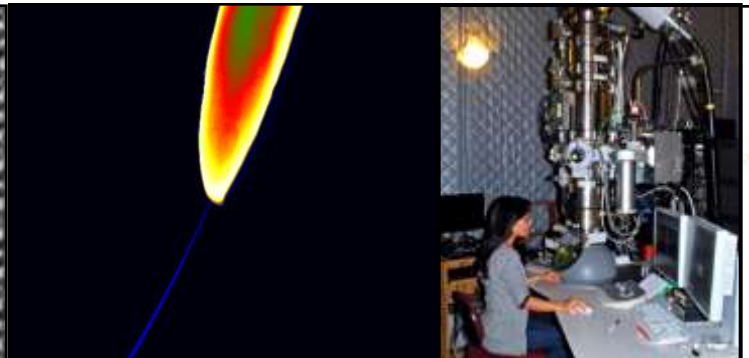


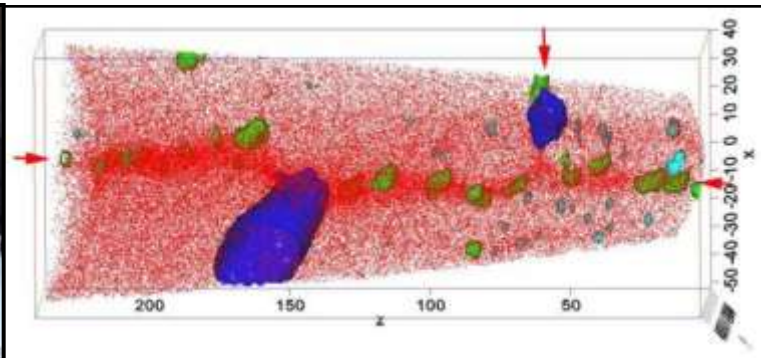


Shared Research Equipment (SHaRE) User Facility

- **BES-SUFD Electron Beam Microcharacterization (EBMC) User Facility with advanced instrumentation and staff expertise to enable world-class materials science research**
- **SHaRE Research Focus Areas:**
  - **μm- to sub-Å-scale materials characterization using analytical and high-resolution *Electron Microscopy* to understand materials behavior**
    - **Catalysts, interfaces, defect analysis, in-situ microscopy techniques, electron tomography, theory/simulation**
  - **Atomic-scale imaging in 3D using *Atom Probe Tomography (ATP)***
    - **Surfaces, buried interfaces, solute segregation, nanoclusters / precipitates, Laser-LEAP extends range of materials for APT analysis (polymer/ceramics/metals)**
  - **Close ties with ORNL BES Programs and User Facilities**
    - **Neutron Science (SNS, HFIR)**
    - **Nanoscience (CNMS)**



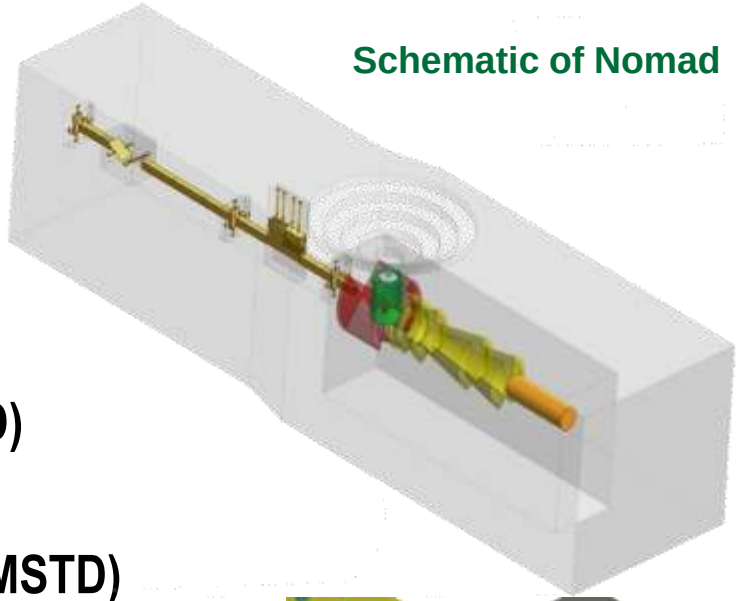


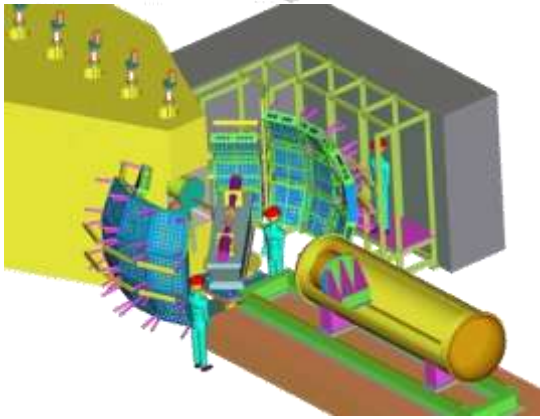


PSD divisions helped lead the development of new SNS/HFIR instruments

- Neutron physics instrument, FPNB (Physics)
- Disordered materials, Nomad (CSD / CNMS)
- Inelastic chopper spectrometer, Sequoia (MSTD)
- Engineering materials diffractometer, Vulcan (MSTD)
- Molecular spectroscopy instrument, Vision (CSD)
- Large molecule diffractometer, LMDI (CSD)
- Small angle neutron scattering, Bio-SANS (CSD)

Schematic of Nomad





Schematic of Vulcan

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Chemical and Material Sciences

- Groundbreaking May 27, 2009
- ARRA funds enabling construction in 2 years rather than 3 years (move spring FY2011)
- Material and labor costs have been favorable; now able to construct extra 20,000 ft^2

Total space 160,000 ft^2

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It's an Exciting Time for Materials R&D at ORNL

- Challenging fundamental scientific issues with strong emphasis on meeting future energy needs
- Vibrant environment
  - Teams of experienced researchers, new hires, collaborating scientists, post-docs and students
  - State-of-the-art-facilities
- Opportunity to expand ORNL's strong history of coupling discoveries based on BES research with energy objectives of DOE's technology programs
- Rapidly expanding work with industry and university partners