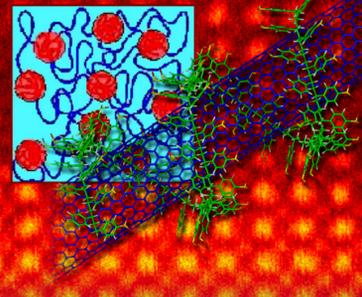


Center for Nanophase Materials Sciences

A Collaborative and Multidisciplinary Center for Nanoscale Science Research under Development at Oak Ridge National Laboratory



The Science

Nanoscience Research on Soft and Complex Materials Combining

Neutron Science Synthesis Science Theory/Modeling & Simulation

Challenges to Synthesis and Understanding

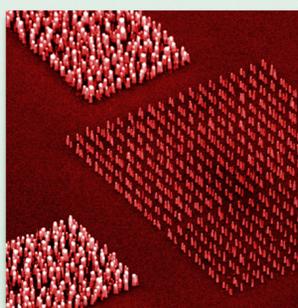
- Control of self-assembly and nanoscale structure
- Understanding how morphology, symmetry, structure, and phase behavior relate to function
- New approaches for rational design and fabrication of soft and hybrid materials
- Choosing the right path in a bewildering array of complex oxide materials
 - More efficient experimental search methods (e.g., nonequilibrium combinatorial synthesis)
 - More intelligent searching (e.g., simulation-driven synthesis)
- Crystals for neutron scattering
 - High-quality bulk single crystals
 - Unique thick-film "superlattice crystals"

Neutron Scattering Opportunities

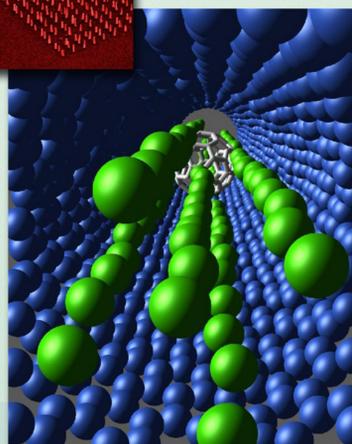
- SANS for nm-scale shape, location, and evolution
- Reflectometry for molecular-scale structure near surfaces and interfaces
- H/D contrast for component-by-component imaging: nanometer to mesoscale
 - "Fillers" to control block copolymer properties
 - Proteins within complexes ("Machines of Life")
 - Atomic-level details for MD simulations
- Dilute and concentrated systems
- Expanded energy, length and time scales

Theory, Modeling and Simulation Opportunities

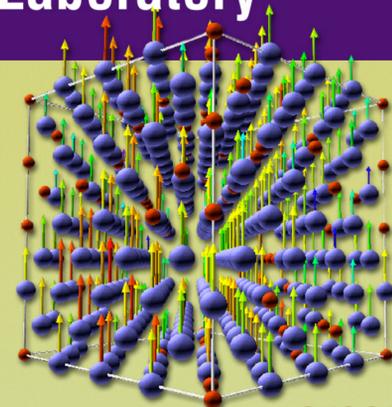
- Nano-magnetism (integrated multiscale modeling)
- Many body methods (correlated electron systems)
- Terascale computing capabilities



Random and ordered arrays of vertically aligned carbon nanofibers, useful for electron field emission and probing into living cells



Computer simulation of a fullerene molecule (white) moving a helium-atom fluid (green) through a carbon nanotube (blue)



Scientific Thrusts

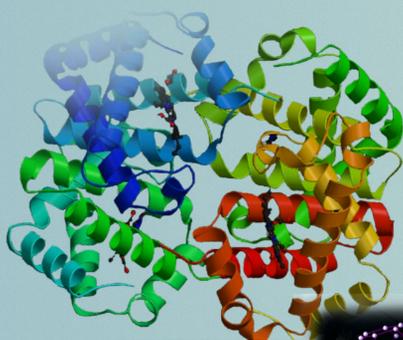
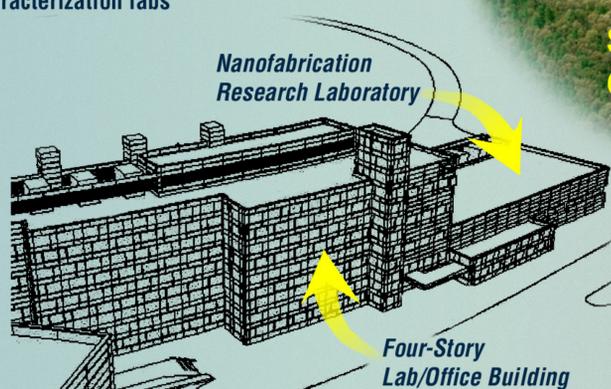
will include research focus areas proposed by the scientific community

- Soft and Hybrid Materials
 - Polymers and biologically derived systems
 - Carbon nanotubes and related structures
 - Nanostructured catalysts
 - Nanoconfined fluids
- Complex Hard Materials: Nanofunctional Materials
 - Nanoscale magnetism
 - Manipulation of collective behavior
 - Effects of reduced dimensionality
 - Quantum transport
 - Structural nanocomposites and nanointerface science
- Nanofabrication
 - Controlled synthesis and directed assembly
 - Link nanoscale phenomena to the macroscale
 - Functionally integrate soft and hard materials
 - Nanofabrication Research Laboratory
- Theory, Modeling, and Simulation: Computational Nanoscience
 - Multiscale modeling
 - Nanomaterials design and virtual synthesis
 - Nanomaterials Theory Institute
- Nanoscale Imaging and Characterization
 - Manipulation of nanostructures for properties measurements
 - Neutron scattering, electron microscopy, scanning probe, and environmental techniques

The Building and Equipment

The Center will be housed in a new 80,000-sq.-ft. facility located on ORNL's Spallation Neutron Source campus

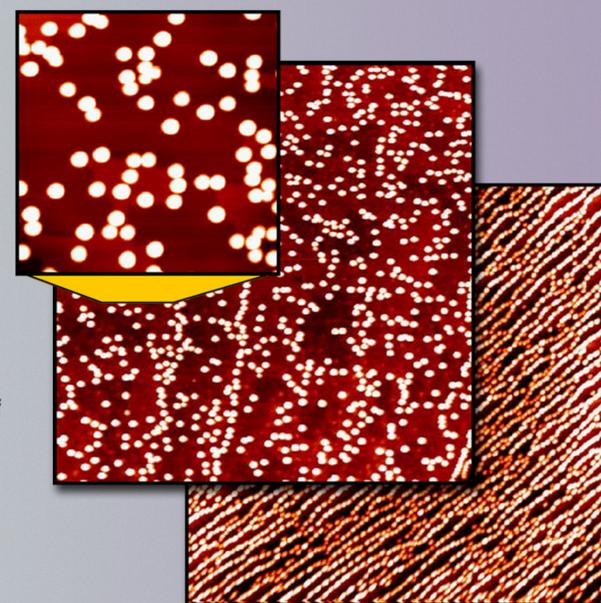
- Office space for core research staff, guest researchers, postdoctoral staff, and graduate students
- Wet and dry materials synthesis and characterization labs
- Nanofabrication Research Laboratory – a 10,000-sq.-ft. clean room facility
- Construction in 2003



Outreach

Half of the Center's researchers will be from universities, industry, and other laboratories

AFM images of Fe nanodots and nanowires on flat and stepped NaCl surfaces (edge length 750 nanometers)



User Program

- Access to state-of-the-art equipment for nanoscale research and engineering
- Vibrant community of research and technical support staff, students, postdoctoral scholars, and collaborating guest scientists
- Program accommodates short- and long-term collaborative research partners
- Access through brief peer-reviewed proposals, with FY03 user activities utilizing ORNL's existing nanoscience capabilities and staff

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