FUTURE SCIENCE NEEDS AND OPPORTUNITIES FOR ELECTRON SCATTERING:

Next-Generation Instrumentation and Beyond

Report of the Basic Energy Sciences Workshop on Electron Scattering for Materials Characterization
March 1-2, 2007

On the Cover:
Characterization of a supported metal catalyst. In multicomponent catalyst systems, segregation of elemental species to active sites enhances activity. Measuring the precise elemental distribution of atomic species on the subnanometer scale is essential to our understanding of how these systems perform and can be optimized. This image is a high-resolution microanalysis map of surface segregation of Pd in nanoscale AuPd bimetallic particles. Pd segregation within the nanoscale particle is shown in green, while Au is in blue. The background support film is carbon.

— *Figure courtesy of C. J. Kiely, Lehigh University.*

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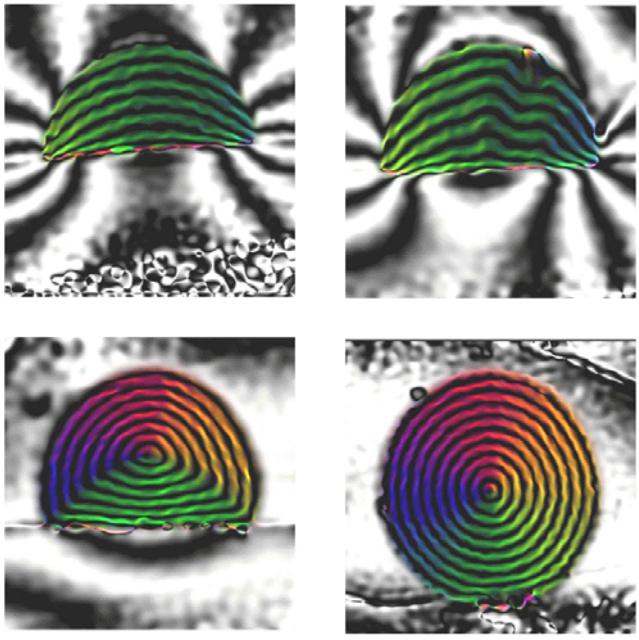

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On the Title Page:
Nanoscale magnetic devices are projected to become a billion-dollar industry in the foreseeable future. Concomitant with the ability to create these novel structures is the need for scientists and engineers to observe and quantitatively characterize these materials. Visualizing and quantitatively measuring magnetic field distributions at the subnanometer level with high sensitivity is only one of the formidable tasks facing scientists in the next decade.

Using a combination of techniques, which include imaging, spectroscopy, and electron holography in state-of-the-art electron microscopes, scientists today can map out the in-plane magnetic field distributions of magnetic structures at resolutions of 10–20 nm. Such measurements are being used to study technologically important questions, such as the coupling of magnetic switching in nanodots or thin films—which have major application in the magnetic recording industry. The challenge for the future is to characterize such fields at or below 1 nm at the highest sensitivity.

The images on the title page illustrate how the magnetic field line flux closure of submicron structures varies as a function of their shape in lithographically fabricated magnetic dots.

Figure courtesy of Nestor J. Zaluzec, Electron Microscopy Center, Argonne National Laboratory, and Rafal Dunin-Borkowski, Cambridge University, UK.

This report is available on the web at http://www.sc.doe.gov/bes/reports/list.html.

CONTENTS

NOTATION

ACRONYMS AND ABBREVIATIONS

BES	Office of Basic Energy Sciences
CCD	charge coupled device
CMOS	Complementary Metal Oxide Semiconductor
DC	direct current
DOE	U.S. Department of Energy
EM	Electron Microscopy
GEN III/IV	generation III/IV
GMR	giant-magneto-resistance
HAADF	high angle annular dark field
HRTEM	high resolution transmission electron microscopy
IR	infrared
MEMS	microelectromechanical systems
R&D	research and development
RF	radio frequency
SEM	scanning electron microscopy or microscope
STEM	scanning transmission electron microscopy or microscope
TEAM	Transmission Electron Aberration-corrected Microscope
TEM	transmission electron microscopy or microscope
UV	ultraviolet
XEDS	x-ray energy dispersive spectroscopy
EELS	electron energy loss spectroscopy

UNITS OF MEASURE

ºC	degree(s) Celsius
µm	micrometer(s)
µs	microsecond(s)
eV	electron volt(s)
fs	femtosecond(s)
Gpixel/s	gigapixel(s) per second
kcps	kilo counts per second
keV	kiloelectron volt(s)
kV/nm	kilovolt(s) per nanometer
mm	millimeters
Mpixel/s	megapixel(s) per second
nm	nanometer(s)
ns	nanosecond(s)
ps	picosecond(s)
sr	steradian(s)

EXECUTIVE SUMMARY

A workshop titled "Future Science Needs and Opportunities for Electron Scattering: Next-Generation Instrumentation and Beyond*"* was held March 1 and 2, 2007, in Gaithersburg, Maryland, to identify emerging basic science and engineering research needs and opportunities that will require major advances in electron-scattering theory, technology, and instrumentation. The workshop was organized to help define the scientific context and strategic priorities for the U.S. Department of Energy's Office of Basic Energy Sciences (DOE-BES) electron-scattering development for materials characterization over the next decade and beyond. Attendees represented university, national laboratory, and commercial research organizations from the United States and around the world. The workshop comprised plenary sessions, breakout groups, and joint open discussion summary sessions. Complete information about this workshop is available at http://www.amc.anl.gov/DoE-ElectronScatteringWorkshop-2007.

SCIENTIFIC CHALLENGES FACING THE CHARACTERIZATION OF MATERIALS

In the last 40 years, advances in instrumentation have gradually increased the resolution capabilities of commercial electron microscopes. Within the last decade, however, a revolution has occurred, facilitating 1-nm resolution in the scanning electron microscope and sub-Ångstrom resolution in the transmission electron microscope. This revolution was a direct result of decades-long research efforts concentrating on electron optics, both theoretically and in practice, leading to implementation of aberration correctors that employ multi-pole electron lenses. While this improvement has been a remarkable achievement, it has also inspired the scientific community to ask what other capabilities are required beyond "image resolution" to more fully address the scientific problems of today's technologically complex materials. During this workshop, a number of scientific challenges requiring breakthroughs in electron scattering and/or instrumentation for characterization of materials were identified. Although the individual scientific problems identified in the workshop were wide-ranging, they are well represented by seven major scientific challenges. These are listed in Table 1, together with their associated application areas as proposed by workshop attendees. Addressing these challenges will require dedicated long-term developmental efforts similar to those that have been applied to the electron optics revolution. This report summarizes the scientific challenges identified by attendees and then outlines the technological issues that need to be addressed by a long-term research and development (R&D) effort to overcome these challenges.

TECHNOLOGICAL CHALLENGES

A recurring message voiced during the meeting was that, while improved image resolution in commercially available tools is significant, this is only the first of many breakthroughs required to answer today's most challenging problems. The major technological issues that were identified, as well as a measure of their relative priority, appear in Table 2. These issues require not only the development of innovative instrumentation but also new analytical procedures that connect experiment, theory, and modeling.

Table 1 Scientific Challenges and Applications Areas Identified during the Workshop

Theme	Application Area
1. The nanoscale origin of macroscopic properties	High-performance 21st century materials in both structural engineering and electronic applications
2. The role of individual atoms, point defects, and dopants in materials	Semiconductors, catalysts, quantum phenomena and confinement, fracture, embrittlement, solar energy, nuclear power, radiation damage
3. Characterization of interfaces at arbitrary orientations	Semiconductors, three-dimensional geometries for nanostructures, grain-boundary-dominated processes, hydrogen storage
4. The interface between ordered and disordered materials	Dynamic behavior of the liquid-solid interface, organic/inorganic interfaces, friction/wear, grain boundaries, welding, polymer/metal/oxide composites, self-assembly
5. Mapping of electromagnetic (EM) fields in and around nanoscale matter	Ferroelectric/magnetic structures, switching, tunneling and transport, quantum confinement/proximity, superconductivity
6. Probing structures in their native environments	Catalysis, fuel cells, organic/inorganic interfaces, functionalized nanoparticles for health care, polymers, biomolecular processes, biomaterials, soft-condensed matter, non-vacuum environments
7. The behavior of matter far from equilibrium	High radiation, high-pressure and high-temperature environments, dynamic/transient behavior, nuclear and fusion energy, outer space, nucleation, growth and synthesis in solution, corrosion, phase transformations

Table 2 Functionality Required to Address Challenges in Table 1

Functionality Required	Priority
1. In-situ environments permitting observation of processes under conditions that replicate real-world/real-time conditions (temperature, pressure, atmosphere, EM fields, fluids) with minimal loss of image and/or spectral resolution	A
2. Detectors that enhance by more than an order of magnitude the temporal, spatial, and/or collection efficiency of existing technologies for electrons, photons, and/or X-rays	A
3. Higher temporal resolution instruments for dynamic studies with a continuous range of operating conditions from microseconds to femtoseconds	A
4. Sources having higher brightness, temporal resolution, and polarization	B
5. Electron-optical configurations designed to study complex interactions of nanoscale objects under multiple excitation processes (photons, fields, ….)	B
6. Virtualized instruments that are operating in connection with experimental tools, allowing real-time data quantitative analysis or simulation, and community software tools for routine and robust data analysis	C

Some research efforts have already begun to address these topics. However, a dedicated and coordinated approach is needed to address these challenges more rapidly. For example, the principles of aberration correction for electron-optical lenses were established theoretically by Scherzer (*Zeitschrift für Physik* **101**(9–10), 593–603) in 1936, but practical implementation was not realized until 1997 (a 61-year development cycle). Reducing development time to less than a decade is essential in addressing the scientific issues in the ever-growing nanoscale materials world. To accomplish this, DOE should make a concerted effort to revise how it funds advanced resources and R&D for electron beam instrumentation across its programs.

INTRODUCTION

PURPOSE OF THE WORKSHOP

A workshop titled "Future Science Needs and Opportunities for Electron Scattering: Next-Generation Instrumentation and Beyond*"* was held March 1 and 2, 2007, in Gaithersburg, Maryland, to identify emerging basic science and engineering research needs and opportunities that require major advances in electron-scattering theory, technology, and instrumentation. The workshop was organized to help define the scientific context and strategic priorities for DOE-BES's electron-scattering development for materials characterization over the next decade and beyond. Attendees represented university, national laboratory, and commercial research organizations from the United States and around the globe. The workshop comprised plenary sessions, breakout groups, and joint open discussion summary sessions. Prior to the meeting, attendees contributed highlights (Appendix C) of issues that they believed represented upcoming science challenges. Presentations of these highlights were used to seed the discussions.

The nation's long-term energy strategy presents many fundamental materials challenges for energy supply, security, and environmental stewardship. DOE-BES has sponsored several workshops to help identify key research issues that must be addressed to meet these challenges. A common theme identified in those workshops is the need for new materials and new tools to characterize them, including, specifically, new electron beam capabilities. To address these issues, this workshop was organized to explore basic research needs as well as new directions to establish where electron scattering will play a critical role. Once these scientific challenges were identified, key new capabilities and instrumentation for addressing these issues were discussed. While current developments in electron scattering, including the DOE TEAM (Transmission Electron Aberration-corrected Microscope) project, are playing a major role in addressing some of these research challenges, the workshop that is the subject of this report sought to look beyond current developments. Through the participation of a cross section of the scientific community, this workshop sought to establish high-priority research directions for electron scattering and instrumentation development in the next decades.

The need for new materials and new tools to characterize them is driven by a range of basic materials issues. Among the DOE-BES workshop reports that identify these needs are *Basic Research Needs for Solid-State Lighting* (2006), *Basic Research Needs for Superconductivity* (2006), *The Path to Sustainable Nuclear Energy: Basic and Applied Research Opportunities for Advanced Fuel Cycles* (2005), *Basic Research Needs for Solar Energy Utilization* (2005), and *Basic Research Needs for the Hydrogen Economy* (2003). (Workshop reports are available at http://www.sc.doe.gov/bes/reports/list.html.) Uniformly, these workshops signal the need for nanoscale characterization with improved spatial and temporal resolution and the capability to characterize materials within their operating environments. For example, the *Basic Research Needs for Solid-State Lighting* report pointed out the need to identify the position and chemical state of each atom in an operating device. Likewise, the *Basic Research Needs for Superconductivity* report highlighted the need to obtain an atomic-level relation between structure and function. The *Basic Research Needs for Solar Energy Utilization* report noted that techniques that combine high spatial and temporal resolution are especially important to resolve elementary physical processes, such as charge trapping, in nanoscale systems. Revolutionary developments in electron scattering are required to address these and other basic research issues.

By providing a forum for discussing how electron scattering can help address these basic research needs and by specifying high-priority research directions for electron scattering and instrumentation development to meet these needs, this workshop facilitated prioritization of resources for the next several decades.

At this workshop, discussion sessions were based on the scientific challenges that might be met by electron scattering, considered in light of (but *not* driven by) current or projected instrumental capabilities, to help prioritize the direction of future development. Input was sought from, and a discussion ensued among, the electron microscopy and broader R&D communities on the full range of needs, capabilities, and opportunities. Discussion sessions focused on three major materials areas: functional materials, nanoparticles, and materials for energy applications. Researchers from around the country and the world with expertise in one or more of these areas, as well as those with cross-cutting expertise in electron-scattering instrumentation and techniques, were invited to attend. The format of the workshop was structured to maximize discussion among the participants, plus DOE representatives (see Appendix B).

CORRELATION OF WORKSHOP THEMES WITH NATIONAL ACADEMY OF SCIENCES GRAND CHALLENGES

In parallel with the DOE-sponsored workshops, a number of meetings organized by the National Academy of Sciences also enunciated the foundations of challenges for the scientific community in the coming decade. The most recent is the report titled *Condensed-Matter and Materials Physics: The Science of the World Around Us: An Interim Report* (Committee on CMMP 2010, 2006). This report identified six major challenges facing scientists over the next decade and suggested that meeting these challenges will lead to "significant advances in both fundamental science and materials-based technology" in the future. These challenges were as follows:

- How do complex phenomena emerge from simple ingredients?
- How will the energy demands of future generations be met?
- What is the physics of life?
- What happens far from equilibrium and why?
- What new discoveries await us in the nanoworld?
- How will the information technology revolution be extended?

Of these grand challenges, a majority map directly onto the thematic challenges developed in this workshop. In particular, both that committee and this workshop identified the important link between the basic knowledge of materials and phenomena and the ability to characterize their constituents.

SCIENTIFIC CHALLENGES AND OPPORTUNITIES

Independent of the application areas addressed during the workshop (functional materials, materials for energy applications, and nanoparticles), the ensuing dialogue among workshop attendees ultimately led to a discussion on the need to understand the nanoscale systems that control materials properties. This report summarizes the essence of these topics and the ensuing discussions, as well as the presentations of the attendees, in seven scientific themes:

- The nanoscale origin of macroscopic properties
- The role of individual atoms, point defects, and dopants in materials
- Characterization of interfaces at arbitrary orientations
- The interface between ordered and disordered materials
- Mapping of electric and magnetic fields in and around nanoscale matter
- Probing of structures in their native environments
- The behavior of matter far from equilibrium

These themes encompass the issues raised by workshop attendees. Each theme is addressed separately in the following sections, which summarize the technological challenges of the associated application areas.

The opportunities for addressing these themes are approaching a nexus. DOE should consider taking the initiative and greatly expanding its role from stewardship of electron-beam characterization facilities to one that rekindles innovation. Procurement for high-end electron-column instrumentation in other countries is nearly triple the amount invested by this country (73% non-U.S. sales, compared with 27% U.S. sales [Mueller, CMMP 2010 Workshop presentation]). This expenditure has mainly been for off-the-shelf commercial instrumentation and tracks with the increased spending and overall rise in funding of nanoscience programs abroad. To respond to this challenge and create an impetus for the United States to regain its lead role in nanoscience R&D, DOE should be taking a bold role in the development of innovative electron optical beamlines for materials characterization. DOE needs to look beyond the present TEAM project, which will ultimately consist of a single resource. Several moderate to high-risk/high-payoff ventures should be added to its portfolio. These ventures, which by their nature will likely operate at the very edges of technology, will be prime opportunities to address a number of the technological challenges proposed by this workshop. Such enterprises should be developed in close coordination with the DOE Electron Beam Microcharacterization Centers, where they should be enabled by long-term research staff and budgets that are sufficient to tackle issues with extended developmental times. The synergies with smaller facilities should not be overlooked; workshop participants recognized that not all developments occur at major user facilities. Therefore, opportunities must also be promoted that can address problems requiring more modest resources, particularly those, for example, involving the development of peripheral components needed to work in concert with resources elsewhere.

SCIENTIFIC CHALLENGE 1. High-Performance Engineering Materials: Understanding the Nanoscale Origin of Macroscopic Properties

Electron beam microcharacterization methods are uniquely suited to improve our insights on how nanoscale phenomena affect the structural integrity of engineering materials under elevated loading (dislocation dynamics, precipitation strengthening, and so on). The challenges are increasing strength, reducing weight, and improving corrosion resistance. Enhancing the performance of engineering materials will reduce infrastructure and transportation costs and increase energy conservation — all crucial components of the long-term solution to the nation's energy needs (Figure 1).

Figure 1 New nanoscale materials will be needed in all aspects of the energy and transportation infrastructure.

Sustainability of the energy supply within the United States is essential. Sustainability must be on a millennial time frame, not decades or even hundreds of years. Therefore, solar, wind, biomass, and geothermal are the only long-term, new options, while nuclear and clean coal may provide a short-term remedy. For new technologies in particular, the energy payback is essential; that is, we must get more energy out than we put in to create the source. A number of these recent technological improvements are evolutionary, and the costs of new energy-related technologies are not coming down fast enough. Revolutions in cost are needed, and new materials, new production methods for current materials, or both provide the pathway to improved performance at lower cost. Detailed fundamental understanding of materials properties under dynamic conditions is a crucial component in bringing about these revolutions, and electron scattering techniques will play a key role in developing this knowledge.

Key Impact Areas

There are numerous cases in which sustainability and efficiency of current commercial technologies are limited by the properties of engineering materials.

For example, classic materials for coal/steam generation (steel boilers and turbine blades) cannot operate at high enough temperatures for highest efficiency. Classic materials for jet turbines for electrical power and aviation (Ni-base superalloys with thermal-barrier coatings) are expensive and rely on some rare, strategically sensitive elements (e.g., Co). Worldwide, corrosion of structural and transportation materials costs $275 billon annually. Hydrogen embrittlement of current alloys can threaten the feasibility of the entire hydrogen economy. Nuclear waste storage is such a politically and environmentally sensitive issue that products must be reprocessed to the point where residual radiation is not a problem. Batteries for energy storage are too expensive

and do not retain charge for long enough, and they use environmentally sensitive materials, so recycling is essential. Better light-emitting diodes and optical band-gap devices, as well as more efficient fuel and solar-cell materials, are needed (Figure 2). Each of these areas is the subject of significant research interest, and electron scattering will play a major role in understanding and improving performance.

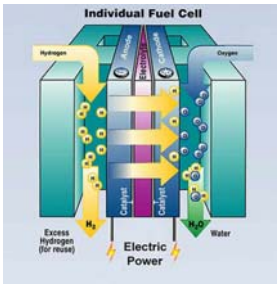

Figure 2 Schematic diagram of fuel cell generating electricity from hydrogen and oxygen.

Summary

These challenges point to new capabilities that must be developed. As pointed out in the executive summary of the *Nanoscience Research for Energy Needs* report (http://www.sc.doe.gov/bes/reports/files/NREN_rpt.pdf), "… all of the elementary steps of energy conversion (e.g., charge transfer, molecular rearrangement, chemical reactions, etc.) take place on the nanoscale." Electron scattering has tremendous capabilities for characterizing structure and composition, with spatial and time resolution. Progress has also been made in controlled environments, including variable temperature and reactive gas and liquid processing (e.g., etching and deposition). We can build on these capabilities and use electron-imaging methods to understand functionality and fundamental processes at the nanoscale.

SCIENTIFIC CHALLENGE 2. When Just a Few Atoms Matter: Understanding Individual Atoms, Point Defects, and Dopants

Solid materials are normally neither pure nor perfect, and often the presence of a small fraction of atoms of a different element or atoms occupying low-symmetry sites profoundly affects materials properties. The unique opportunity for electron-beam nanocharacterization is not only to investigate the average effects of impurities and defects, but also to probe properties of individual atomic-scale features. An important grand challenge in electron microscopy has been atomic-resolution imaging of individual point defects, and we are beginning to see examples where this goal can be achieved. We now have the opportunity to generalize these encouraging results:

- Can we image, localize, and characterize single (dopant, impurity) atoms and single point defects (vacancies/interstitials)?
- Can we achieve subnanometer (or better) resolution and sensitivity in a thick (10 μm) specimen of real material in an ambient environment?
- Can we extend this to measuring the local behavior of single electrons?

These questions need to be answered to solve compelling problems in energy generation and storage, environmental catalysis, structural materials, and functional materials (such as semiconductor devices). There are numerous cases in which the properties of current and future commercial products are limited by the presence of very small amounts of (or even single)

impurity/dopant atoms or crystal defects, and measuring the distribution of different elements (Figure 3) is an important challenge. In terms of mechanical properties, the embrittlement of otherwise ductile metals and alloys by local segregation of trace amounts of impurities (e.g., Al by Ga, Cu by Bi, Fe by S and P) is an important example — it is an industrial-scale materials processing issue, translating into billions of dollars spent to remove undesirable impurities (e.g., from pressure-vessel steels). Equally important and poorly understood is the specific role of hydrogen in destroying the mechanical properties of many engineering materials. Many high-performance engineering components, such as jet turbine blades, depend on the deliberate addition of trace amounts of specific elements to create desired bulk materials properties.

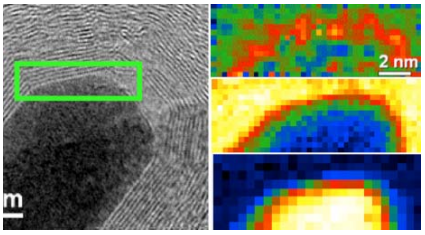

Figure 3 (right) Maps of different atomic layer segregants to the (left) surface of a nanotube.

The semiconductor industry is essentially based on the ability to control and understand trace impurities and defects. Desired electrical properties of semiconductors depend on successfully putting dopant atoms in the right places, while the presence of small amounts or even single atoms of the wrong element can destroy the properties of a semiconductor device.

Corrosion and catalysis are large-scale challenges in which the chemical activity of materials often depends on control over the distribution of single atoms or groups of atoms on a surface or support substrate. For example, deliberate dispersal of elements or compounds can produce novel catalyst materials and transform the properties of the same material in bulk (e.g., inert bulk Au becomes an active catalyst when dispersed in sufficiently small particles).

Single-Atom Sensitivity: Current Limits, Future Opportunities

Imaging the structure of planar and linear crystal defects with atomic resolution by electron-scattering methods is a mature field. It is becoming possible to identify the nature of single isolated atoms on thin substrates and also the nature of single impurity/dopant atoms within crystalline matrices of other atoms.

Measuring the position (in three dimensions) and the elemental nature of individual atoms will soon be more generally possible. Beyond three-dimensional atomic-resolution imaging, it will be important to explore how electron-scattering techniques can be extended to detect the chemical bonding and the electrical and magnetic fields of individual atoms. For example, the development of electron-based tomographic spectroscopy may allow three-dimensional structure with chemical contrast (Figure 4). Can the influence of specific atoms on the physical and chemical properties of materials be measured? Can sensitivity be improved to the point at which changes in electrical and other properties may involve the actions of single electrons or the transfer of charge of < 1 electron? Moreover, an important

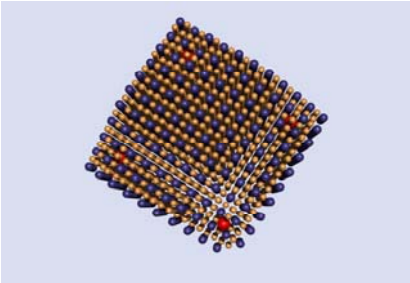

Figure 4 Atomic-resolution x-ray and electron spectroscopy, as well as imaging using electron-scattering-based techniques, will be required for true single-atom analysis.

challenge will be to extend single-atom sensitivity to nonplanar/inhomogeneous interfaces in real materials and ultimately to noncrystalline and amorphous materials.

Finally, the success of these advances in electron-scattering methods is strongly coupled with theoretical and computational capabilities. Modeling the phenomena that can be observed experimentally and predicting the effects of atomic-scale defects on materials properties is a crucial key to the creation of novel materials/materials systems.

Summary

Materials for catalysis, materials for power generation (nuclear, coal), materials for energy storage and transportation (hydrogen), materials for renewable energy (solar), and functional materials are all affected (positively and negatively) by trace amounts (down to the single-atom level) of specific elements and the presence of specific crystal defects. The next generation of electron-scattering instruments needs to be able to *locate precisely and characterize completely* single atoms in real materials

SCIENTIFIC CHALLENGE 3. Turning the Corner: Interfaces at Arbitrary Orientations

Most materials are composed of smaller distinct building blocks. The behavior of interfaces — the boundary region where these building blocks meet — can have a significant impact on the behavior of a structure as a whole. For example, the structural integrity of a wall depends not only on the properties of its building blocks of brick or stone, but also on the properties of the mortar that joins them. As the scale of structural units becomes smaller, an increasing volume fraction of the structure is tied up in these interfaces, and the influence of interface properties becomes correspondingly larger. In the limit that the dimensions of the building blocks approach the nanometer scale, as in the case of the transistors in current-generation computer chips, the material behavior may show little resemblance to the "bulk" macroscopic properties.

Scientific understanding of interfaces is in its relative infancy. The host of methods devised during the 20th century to improve understanding of free surfaces — from X-ray scattering and spectroscopy to scanned probe microscopies — are not generally applicable to the study of interfaces. In particular, it is necessary to "see into" the material to probe interfaces, which do not have the easy accessibility of free surfaces. Electron scattering methods are ideally suited to this task and have already made tremendous contributions to characterizing the local atomic configurations, composition, and electronic structure of interfaces. However, these contributions have been largely limited to "special" interfaces that exhibit high symmetry in projection because of the low numerical aperture of electron optics. In effect, we have been able to learn a great deal about interfaces that are flat and parallel like the mortar in a brick wall, but interfaces with the complex and variable geometry of the stone wall elude us (Figure 5). And the world of nanotechnology is not made of "bricks": the transistors that will power electronic devices a decade down the road will depart from the traditional layered geometry, taking on complex three-dimensional geometries (Figure 6). As a result, the extension of interfacial characterization

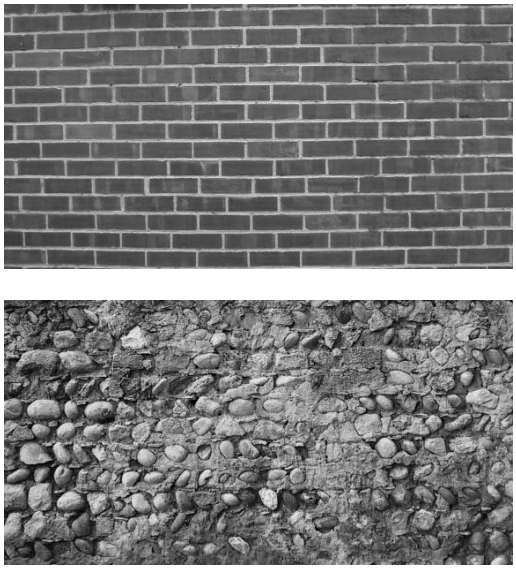

Figure 5 Transmission electron microscopy (TEM) has made excellent contributions to the understanding of "special" interfaces, where flat parallel grains merge, like the mortar in a brick wall. Substantial work is needed for similar understanding of complex three-dimensional interfaces, like the mortar in a stone wall.

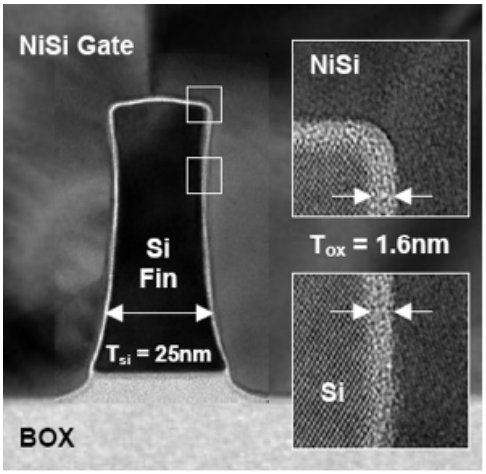

Figure 6 Nanostructure equivalent of the stone wall: TEM image of a FinFET, the transistor that will sustain improvements in computing power a decade from now. The gate dielectric layer that separates the single-crystal Si fin from the NiSi electrode has an arching three-dimensional geometry and is just 1.6 nm, or a few atomic diameters, thick.

to arbitrary three-dimensional geometries will be required to fully understand the operation and reliability of these devices.

The formation of complex three-dimensional interfaces is not limited to structures such as those manufactured for the microelectronics industry. These interfaces are ubiquitous in natural processes of scientific and technological importance: between catalyst particle and support in catalytic converters, between fluid and membrane in fuel cells, between nanoparticle and macromolecule in advanced drug delivery systems, between core and shell in bimetallic nanoparticles, or between scale and alloy during the early stages of oxidation or corrosion. Complex three-dimensional interfaces are characteristic of such important dynamic processes as deformation in crystals, phase transformations, and the catalytic growth of carbon nanotubes and semiconductor nanowires.

Moreover, this gap in understanding inhibits the critical link between structure and behavior from being uncovered. To make this link, the interfaces that control properties must be *representative* of the material; this will never be the case as long as studies are limited to those "special" interfaces conveniently well-suited to the limitations of measurement methods. How does a change in the plane of a crystal boundary affect local composition (i.e., solute segregation) and electronic structure? How does this chemical variation thereby influence physical and mechanical properties, such as interfacial strength, or the ability to transmit a superconducting current? How does the three-dimensional motion of ledges on two-dimensional

planar interfaces or jogs on one-dimensional dislocations control deformation in crystals? How does the three-dimensional nature of an internal interface affect internal strain and thereby mechanical toughness in a structural material or the mobility of charge carriers in a transistor? These questions can be answered only with the development of next-generation techniques that allow the characterization — structural, compositional, and electronic — of interfaces at arbitrary orientations.

SCIENTIFIC CHALLENGE 4. Order and Disorder: Crystals Interacting with Liquids, Vapors, and Soft Materials

The role of interfaces in governing physical properties and dynamic behavior of materials is omnipresent. Electron-scattering techniques have been very successful in providing important contributions toward understanding solid-solid interfaces. Also, in areas focusing on noncrystalline materials, particularly in the life sciences, microscopy has made a strong impact. However, tremendous opportunities exist where only the first small steps have been taken; interfaces where crystals are in contact with less ordered states of matter have remained a challenge.

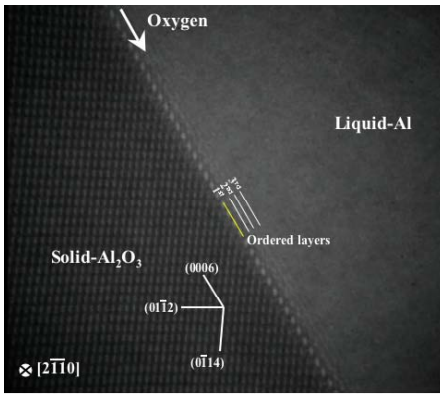

Figure 7 HRTEM image of the interface between solid Al_2O_3 and liquid Al (Source: Ruehle, workshop participant).

Understanding solid-vapor, solid-liquid, and hard-soft interfaces is the key to progress in a number of important fields, including energy conversion, catalysis, the life sciences, electronics, and engineered materials.

Advancing a Broad Spectrum of Research

The importance of interfaces between crystalline and noncrystalline materials is enormous. For example, electrolytic processes and corrosion are fundamental phenomena that take place at solid–liquid or solid–gas interfaces. Many energy-conversion problems, ranging from battery technology to fuel cells and catalysis, depend on interface phenomena at boundaries between crystalline and noncrystalline phases. Polymer-nanocrystal hybrid photovoltaic materials are currently under development and show great promise. Investigations of atomic-scale processes *during* the growth of electronic materials (rather than *postmortem*) and of the nature of interfaces between traditional semiconductor materials and novel applications of polymers are needed. Biochemical processes are fundamentally controlled at interfaces that usually do not possess crystalline order. Intergranular glassy films profoundly affect the properties of structural ceramics. Joining technologies, including soldering, welding, and adhesive bonding, as well as the science of friction, wear, and lubrication, all depend on interfaces between ordered and disordered materials. *Can we study these features at atomic resolution?*

Details of the atomic-level phenomena taking place at interfaces between crystalline and disordered matter change physical properties in the near-interface regions. Proximity effects

often crucially impact the materials on both sides of the interface: interaction with liquids can affect atomic reconstructions on the crystalline side of an interface while, conversely, enhanced short-range order can be seen in liquid layers next to a crystal (Figure 7).

Nearly every material was formed, at some point, through either condensation or dispersal of matter at interfaces between solid and liquid, gaseous, or otherwise disordered phases (Figure 8). Electron-scattering techniques should be extended to the *simultaneous* investigation of crystalline and disordered material in contact, in atomic detail. Meeting this challenge appears feasible and will provide major advances in a broad spectrum of fields.

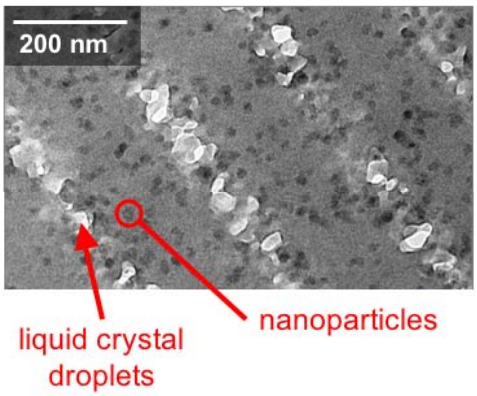

Figure 8 Polymer/crystal interface in nanocomposite materials (Source: Braun, workshop participant).

Key Technique Development Areas

Electron-scattering methods can spatially resolve the first few atomic layers that control interface properties while providing a host of signals to resolve electronic, chemical, optical, and many other physical properties. Combined with theory, modeling, and simulation, these methods will allow us to understand and ultimately engineer interfaces.

Important opportunities exist for improving experimental methods to meet diverse needs for probing these classes of systems. Providing physical environments inside microscopes such that noncrystalline materials remain in their native states is a rapidly growing field. Much room for improved capabilities remains for both high-temperature and cryogenic specimen stages. In-situ cells to contain liquids or gases and image how they interact with solids are currently becoming reality and are beginning to provide key insights, for example, in the area of electrochemical etching and deposition. Simultaneously optimizing for different mechanisms of image contrast formation is an important issue. Imaging conditions can be optimized to observe crystalline structures *or* to image "soft" matter. Imaging techniques that provide good contrast on both sides of hard–soft interfaces remain a challenge. Using microelectromechanical systems (MEMS) techniques to construct suitable phase plates may be one feasible approach.

An issue inherent to electron microscopy is the possibility that samples may not remain unchanged in the presence of the electron beam. "Beam damage" mechanisms are different in crystalline then in soft materials; hence, optimized operation conditions for studying hard–soft interfaces must be carefully balanced.

Specific Experimental Opportunities

Perfecting methods for in-situ electron-beam investigation of reactions at solid–liquid and solid–vapor interfaces impacts numerous manufacturing processes.

Generalizing the ability to image atomic mechanisms of heterogeneous catalytic reactions remains an important challenge. For example, imaging the environmental dependence of catalyst particle three-dimensional morphology, observing the transport of reactants, and understanding the role of support structures and ensemble effects are all areas where electron-scattering methods are just beginning to reveal their potential benefit. With assembly processes in solution-based nanosystems becoming widely used, the ability to visualize the underlying atomic-scale phenomena is an important basis. Atomic-resolution observation of diffusion and transport in multicomponent systems, visualization of nucleation events, and direct imaging of chemical ligands may be possible with the help of optimized instrumentation. Similarly, all elementary processes of energy conversion occur at the nanoscale. A better understanding of these processes could be achieved if new capabilities for imaging charge transport/transfer, molecular rearrangement, and chemical reactions can be developed.

In the life sciences as well as in other fields, including electronics, being able to visualize nanoscale amorphous and nanocrystalline materials with interface specificity is a crucial goal. Can we achieve atomic-level imaging of proteins, cells, viruses, and nano-bio composites while maintaining them in their natural states? How might we detect and quantify functional components and interactions with drugs, targeting agents, and imaging agents? Seventy percent of drug molecules interact with membrane proteins, most of which cannot be crystallized; thus, solving the structure of proteins that cannot be crystallized by imaging individual proteins via real-space and reciprocal-space methods is an unmet and valuable challenge. The priority developments identified in this workshop will provide a pathway toward understanding many of these issues.

SCIENTIFIC CHALLENGE 5. Mapping of Fields in and around Matter

The influence of applied fields on materials and the role of internal fields in materials behavior are key to many advanced technologies, yet our capabilities for studying how these fields interact with matter through electron scattering are relatively limited. Smart cards based on ferroelectric memory are used for security and identification as well as a wide range of personal applications. Magnetic materials are ubiquitous in computing applications, providing the primary means of data storage. The operation of most processors is based on switching of local electric fields, and the development of magnetic tunnel junctions for random access memory is being extensively pursued. Motivated by these applications, workshop participants viewed improving the understanding of the interaction between applied and internal fields with microstructure as a major challenge and opportunity.

Electron scattering and microscopy provide new opportunities in several key areas: understanding domain reversal mechanisms and tunneling processes, understanding vortex dynamics, achieving imaging and quantitative measurement of fields with better resolution, extending imaging and quantification to three dimensions, correlating local fields with crystal structure, and visualizing the dynamic processes of field penetration and redistribution. Workshop participants agreed that advancing the capability for addressing these issues through electron scattering should be a high priority for DOE-BES.

Scientific Opportunities

Exploring Magnetism, Spin, and Exchange Interactions by Electron Scattering

Magnetic behavior is governed by magnetic exchange interactions that determine how spins are arranged in a material and how they interact. Controlling these exchange interactions in magnetic nanostructures is key to many modern achievements, such as giant-magneto-resistance (GMR). Although theory and modeling have provided many predictions of behavior based on exchange coupling, the length scale of magnetic exchange interactions typically is a few nanometers, and magnetism or spin has not been directly imaged below the 1-nm level using electron scattering to date.

An example of this challenge is in the drive to increase the capacity of magnetism-based data storage. This need has led to the development of materials with ever-smaller magnetic domains and ultimately bit-patterned media. As the size decreases, exchange interactions and magnetostatic terms become more dominant in the overall energy of the system. The magnetic structure and interactions in these materials are difficult to study because imaging of nanometer-scale domains and within domain walls is beyond the present capability of electron scattering. Atomic-resolution imaging of spin has been achieved at surfaces through spin-polarized scanning tunneling microscopy (Figure 9). Can electron microscopy achieve high-resolution magnetic imaging in volumes of materials?

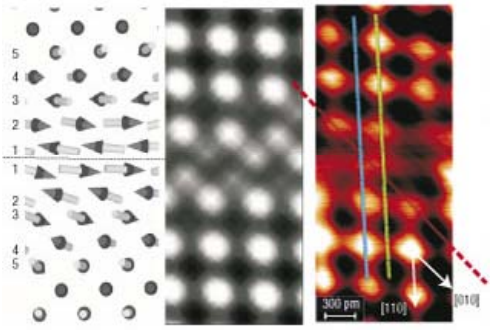

Figure 9 Atomic-resolution imaging of spin at a surface using scanning tunneling microscopy (Source: Bode et al., 2006, *Nature Materials* **5** 477–481).

Achieving high-sensitivity imaging through electron scattering could help to address many scientific challenges raised at the workshop. The structure and interactions in nanodomain materials could be measured and evaluated against models. The structures of new materials, such as multiferroics and heterostructures, could be explored and understood. Ultimately, with sufficient resolution, the structure inside domain walls or defects in antiferromagnetic structures could be resolved. An opportunity presented at the workshop is to use a spin-polarized electron source in an electron microscope, which could lead to more powerful imaging capabilities using linear or circular magnetic dichroism, for example. These approaches provide new opportunities to study nanoscale magnetic features through the thickness of a material to complement the existing scanning-probe microscopy and X-ray-based approaches (Figure 10).

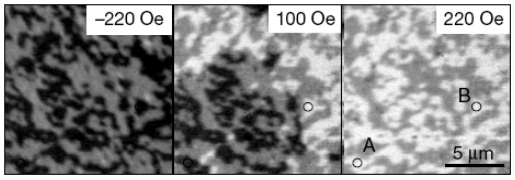

Figure 10 Images of the domain structure in Co using X-ray magnetic circular dichroism (collected in zero field) following application of the applied field indicated (Source: Nolting et al., 2000, *Nature* **405** 767–769).

Real-World Challenges — Three-Dimensional Field Mapping

While many of the applications for magnetic materials rely on two-dimensional structures, surface boundary conditions lead to complex arrangements of spin. Likewise, similar effects play a strong role in electric field distributions near surfaces in ferroelectric materials.

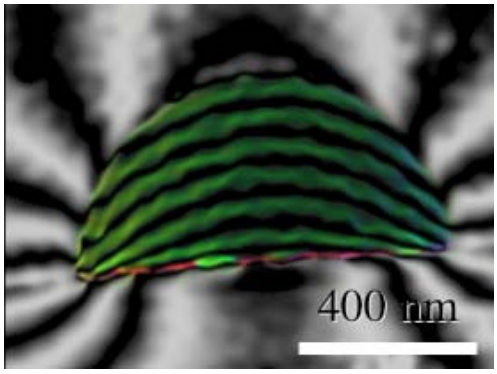

Figure 11 Magnetic field lines surrounding an individual lithographically fabricated nanostructure in two dimensions (Source: Zaluzec, workshop participant).

Even in the smallest of nanoparticles, field distributions are complicated, influenced by the external applied field (Figure 11), the internal structure of the particle, and the fields associated with nearby particles. Consequently, beyond improving resolution to map fields in two dimensions, we would like to achieve mapping in *three dimensions*. A rationale for this goal is that all materials have surfaces that can influence field distributions. Indeed, a compelling case is made for electron scattering, considering that such studies require very thin samples in which surfaces can dominate behavior. To make the connection to real-world materials that often have larger dimensions, three-dimensional mapping using electron scattering will play an important role.

There are many important issues that can be addressed, but one intriguing challenge raised at the workshop is related to the three-dimensional arrangement of magnetic vortices in a superconductor. The properties of superconductors depend strongly on the pinning of these vortices, each of which contains one quantum of flux, that form in Type II superconductors under applied magnetic fields (Figure 12).

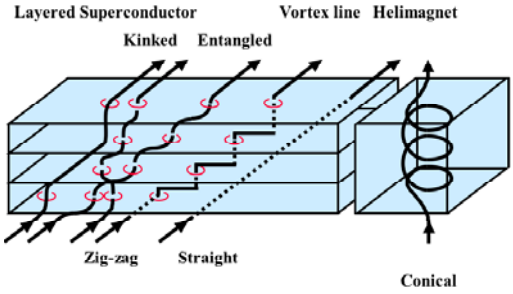

Figure 12 Three-dimensional arrangements of superconducting vortices (Source: Tonomura, workshop participant).

Significant improvements in our knowledge of vortex interactions have been gained from imaging of vortex configurations (Figure 13). Imaging of vortices using microscopy offers advantages over scanning tunneling techniques because the latter approach is sensitive only to surface fields generated by the vortex. Electron microscopy offers perhaps the only opportunity to map the vortex distribution in three dimensions because there is the possibility of imaging a vortex along its length. However, significant improvements in field resolution while precisely controlling the field at the sample are needed, together with the development of tomographic methods for magnetic imaging.

Linking Crystal Structure and Defects to Local Fields

A significant challenge raised at the workshop is the correlation of microstructural features with local field perturbations. A good example is the case of vortices in superconductors, described above. A major challenge is to identify the microstructural features that pin the vortices (Figure 14). At present, this is very difficult to accomplish because of the limitations in performance of microscopes operating in a field-imaging mode.

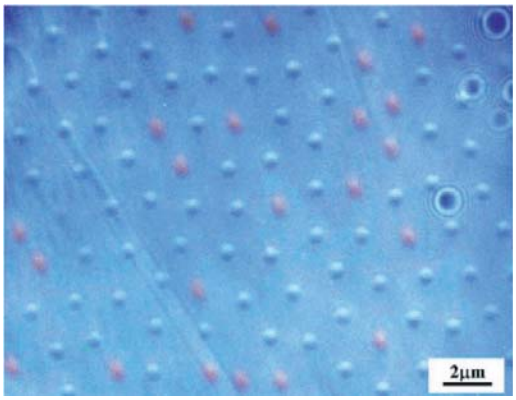

Figure 13 Lorentz micrograph of vortices in high-T_c Bi-2212 superconducting thin film with tilted columnar defects. The red-vortex images correspond to vortices trapped at defects (Source: A. Tonomura, 2006, *Proc. Jpn. Acad., Ser B* **82** 45–58).

Imaging of local fields by either holographic interference techniques or Lorentz microscopy typically involves working under conditions for which imaging of structure is limited by the magnetic induction of the lenses. Consequently, it is challenging to make a direct correlation between local fields and local structure. To identify a defect that may be pinning a vortex, for example, a Lorentz image of the vortex must first be obtained and then, under very different conditions, an image of the structure collected. However, with present Lorentz imaging lenses, the resolution for structural imaging is rather poor compared to imaging under non-Lorentz conditions. Significant opportunities to improve resolution under these conditions by utilizing aberration correction were of considerable interest at the workshop.

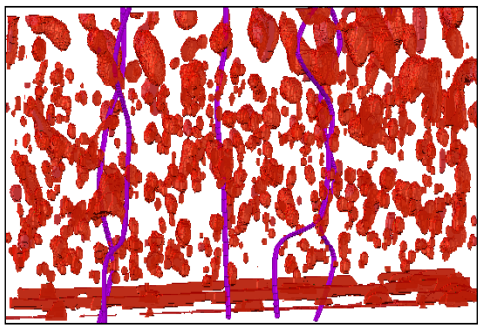

Figure 14 Schematic representation of simultaneous imaging of structure and vortices, revealing how vortices may be pinned at defects (Source: Miller, workshop participant).

Domain Dynamics

Beyond simply mapping field distributions in solids at high resolution, it is equally important to understand the dynamic behavior under changing electric/magnetic conditions. For many areas of materials investigation, developing new capabilities for in-situ science in the electron microscope was a strongly supported topic at the workshop, and in-situ studies can play a large role in improving the understanding of how fields interact with matter. For example, a major challenge discussed at the workshop related to how field redistribution is influenced by microstructure and defects in a material. Addressing this issue will require developments to improve resolution for imaging of both fields and structure at the same time, as described above, but novel approaches to introduce appropriate fields at the sample and to accommodate the influence of those fields on the electron beam path also need to be developed. The strong view of workshop participants is that these areas should be pursued aggressively by DOE-BES.

Key Technical Challenges

The scientific opportunities described above present many technical challenges for electron scattering that could be addressed in the BES portfolio. Key technical challenges are imaging structure at an atomic level and magnetic behavior at the same time and achieving nanosecond time resolution (or better) for observing switching processes. Underlying many of the scientific opportunities presented at the workshop is the need to be able to introduce the appropriate environment in the microscope at the sample. In the case of mapping fields around materials, improved control of fields at the sample location is of great importance. Priority research and development directions for electron scattering should address these challenges.

SCIENTIFIC CHALLENGE 6. Small Particles — Large Impact

The role of small particles, both natural and man-made, continues to dominate chemical, mechanical, and electrical processes in a wide range of today's science applications. Both equilibrium and non-equilibrium systems are now being fabricated at scales spanning the range from submicron to subnanometer dimensions. However, the mechanisms and/or sites that these small particles control, as well as how the particles themselves form and interact, remain key scientific challenges.

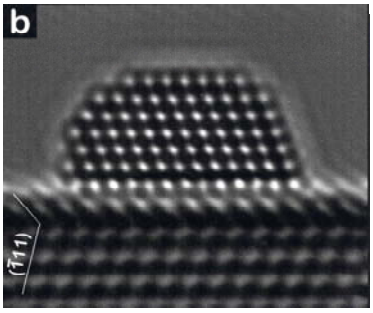

Figure 15 Calculated HRTEM image of a Rh catalyst on CeO_2 support (Source: Kiely, workshop participant)

Scientific Challenges

Although the key issues vary depending upon the application of a particular small particle, the questions that the research community asks about small particles remain remarkably consistent: Where is every atom in the particle? How is each bonded to its neighbors? What is that atom's relationship to the process at hand? Are there site-specific regions that influence properties? How do external factors affect these sites?

Nucleation, growth, and assembly play the dominant roles in synthesis of small particles. The issues that dominate this field amount to (a) what controls the initial nucleation event and (b) how the particles evolve from their initial to their final states. The simplest example of this is single-phase nanoparticle creation and growth from solution or vapor. The majority of structural evolution studies are not performed during the growth process, but rather after the fact; postmortem or time-sliced observations are performed and a sequence of events is reasonably postulated. This procedure is suitable for simple systems, but more complicated cases, such as metamaterials (which are formed by the interaction of soft organic ligands with a traditional metallic or oxide matrix) remain challenging. In particular, the near-real-time observation and measurement of individual nanoparticle formation from the glassy to crystalline state, where diffusion and transport in multicomponent systems are controlling factors, are essential to understanding mechanisms that drive synthesis in non-equilibrium and artificially created materials.

Catalysts and their associated reactions are of paramount importance to the modern chemical industry (Figure 15). It is estimated that more than 50% of today's products involve catalysis in some stage of their manufacture. This multitrillion-dollar industry is an essential component of the ability to create both day-to-day consumer products and new materials by lowering the activation energy for a transformation or conversion process. A large fraction of catalysts are by their very nature small particles (Figure 16). While many catalysts used in industry today are regenerated and used multiple times, a number are single-use products that are complex to fabricate, occasionally toxic after reaction (resulting in high disposal costs), or overly reliant on expensive raw materials such as platinum and rhodium. Thus, the need for optimization is profound. To accomplish this feat, the key parameters that researchers need to identify are (Figure 17):

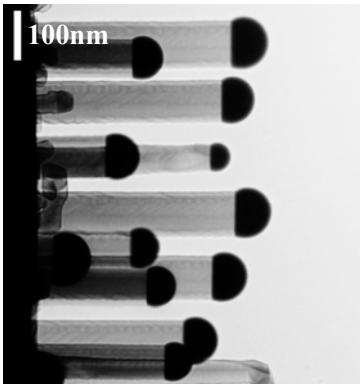

Figure 16 Nanowires grown in situ. The three-dimensional shape and the composition of the catalyst and wire have not been determined during growth (Source: Ross, workshop participant).

- The location and analysis of active sites as well as the reactant
- Three-dimensional structure and composition profiles of the particles under near-reaction conditions
- Surface structure in the presence of reactants
- The state (dispersion, morphology, valence) of supported particles and adjacent areas under catalytically relevant redox cycles
- Dynamics of catalyst-support interactions
- Species transport within a catalyst structure during reactions
- Visualization of the absorption/desorption processes

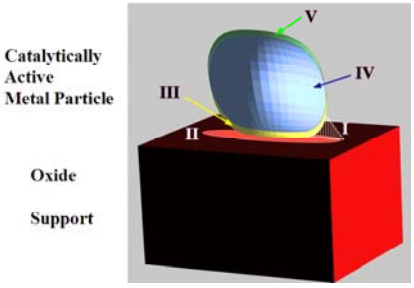

Figure 17 Site-specific locations for catalysis (Source: Disko, workshop participant).

An emerging area of small-particle research is in the regime of soft nano-bio particles. Here the challenge is similar to the problems delineated above; however, the complications are the detection and quantification of the functional organic components attached to individual nanoparticles, such as the tridentate complex (Figure 18). This is particularly important when these soft multifunctional particles and their organic ligands are loaded with drugs, targeted agents, or imaging agents (for use in cell and tissue imaging). The problem can be restated as: Can proteins, cells, viruses, and nano-bio composites be imaged at the atomic level while being maintained in a natural state with physiological viability?

Technical Challenges

The technical challenges to answering these issues are more than a simple task of improving image resolution. The following areas were identified as critical capabilities that should be developed:

- Atomic resolution in controlled environments of temperature, pressure, and liquid conditions, with precise control and monitoring of the gases and/or liquid flow
- Simultaneous high-efficiency spectroscopic mapping/ analysis techniques that operate under these conditions
- Time-resolution capabilities in order to study the progress of chemical reactions
- Development of analytical techniques to image organic ligands connected to metamaterials
- Development of in-situ and ex-situ cells compatible with the next generation of instruments, particularly those that enable applications of EM fields, light, and chemical potential as external driving forces for nucleation, assembly, and growth.

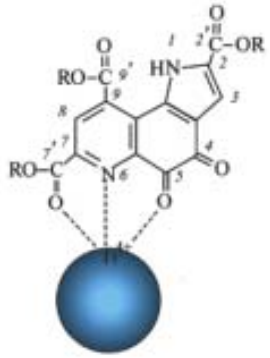

Figure 18 Tridentate complex of Ti on a TiO_2 nanoparticle with pyrroloquinoline quinone (Source: Dimitrijevic et al., 2006, *J. Phys. Chem. B* **110**[50], 25392–25398).

SCIENTIFIC CHALLENGE 7. Materials in Extreme Environments: The Behavior of Matter Far from Equilibrium

The challenge of studying the local structure of materials at the atomic scale in extreme environments represents one of the most difficult tasks for electron scattering. One of these challenges rests implicitly within the instrumentation, since in a conventional implementation the electron microscope is, for some materials, an extreme environment due to its internal high vacuum and thus in itself creates a nontrivial technical challenge to be redressed in the near term.

Today's engineering materials are exposed to environmental states as varied as there are applications. High temperature and/or pressure, radiation, EM field gradients, and the presence of gaseous or fluidic media represent the breadth of conditions under which modern materials systems are fabricated, transported, stored, or operated. At present, there is no instrument that can successfully interrogate the structure of individual subnanometer regions under conditions that replicate such real-world conditions.

The scientific challenges are many. For example, in the power arena, predicting the performance of materials as well as subsequent waste forms during both operation and ensuing disposal or storage is essential for the safe and economic operation of next-generation energy resources. These issues are pervasive regardless of whether fission, fusion, solar, hydrogen, or hydrocarbon combustion is used for energy generation. Materials performance is directly coupled to their microstructure and composition (Figure 19).

To design and/or characterize the radiation resistance of new materials for use in Gen III and IV nuclear reactors, it is of paramount importance to characterize the roles of site-specific interfaces between precipitates and the matrix and the formation of defect clusters, and to determine how individual defects facilitate elemental transport under conditions of high radiation exposure at pressure and temperature. At present, irradiation environments are simulated either by high-energy-particle irradiation, in which medium-resolution observations are performed at temperature, or through postmortem analysis of defect structures. In either case, it is necessary to postulate the transport processes that occur between the initial and final states, as well as to hypothesize the mechanisms of failure. The ability to observe and quantitatively measure in-situ irradiation-induced atomic transport will provide invaluable insights into the mechanisms that control performance.

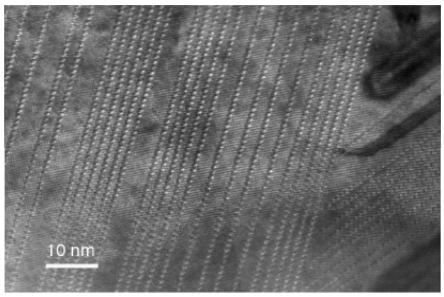

Figure 19 Extended planar defects in a ceramic waste form, which may facilitate elemental transport in reduced rutile (Source: Smith, workshop participant).

In the non-nuclear regime, comparable issues abound, and the absence of irradiation is an additional contributing factor. For example, the ability to elucidate the mechanisms of charge transfer in fuel cells or photovoltaics during energy capture, conversion, or transport at the nanoscale under steady-state conditions would provide essential information on operation, as well as on mechanisms controlling their degradation and failure (Figure 20).

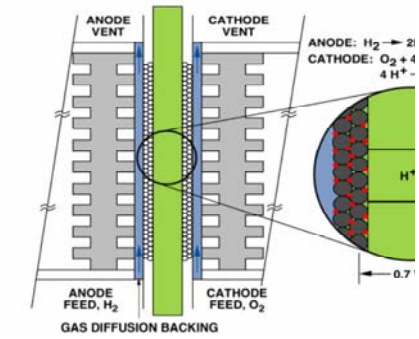

Figure 20 Cross-section of fuel cell (Source: J. Turner, workshop participant).

In catalysis, there is very little knowledge of how three-dimensional morphological transformations proceed within fuel cells or during petrochemical processes as a function of temperature and pressure. Critical to the design and optimization of catalysts is a knowledge of the physical extent of the active sites on a catalyst and/or its support as well as how active species are transported to particles to effect the various reactions. How these vary and in what manner are fundamental questions that have never been answered with real-time, in-situ measurements at the atomic level. Such correlations between nanostructure and activity are necessary to determine the fundamental chemistry in heterogeneous catalysis (Figure 21).

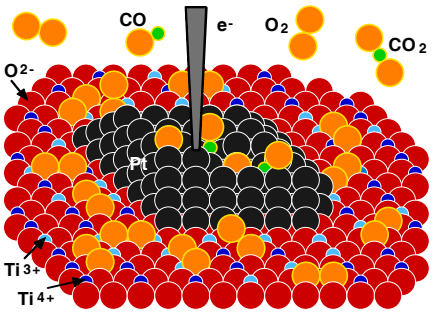

Figure 21 Illustration of atomic-level site-specific analysis of Pt/TiO_2 catalyst system (Source: Anderson, workshop participant).

Corrosion in all its manifestations is a dead weight on materials, having at times huge economic ramifications. The recent failure of the Prudhoe Bay pipeline, which carried 650,000 barrels of crude oil per day, is a direct result of corrosion. In-situ microstructural and microanalytical

studies would provide key information to understand and ultimately control this deleterious condition.

Finally, this period is frequently called the Silicon Age, notwithstanding the fact that we are organic carbon-based life forms. A huge investment in creating organic/inorganic interfaces is beginning; however, we do not have the ability to image proteins, cells, viruses, or these new nano-bio composites at the atomic level while maintaining their natural state and/or physiological viability. Some progress has been made in our capability to image materials at high resolution in an aqueous environment (Figure 22), but the key challenges require much higher resolution. The development of in-situ capabilities that permit the atomic-resolution observation and characterization of organic/inorganic interfaces and structures in a liquid suspension will be a complex and immensely challenging proposition.

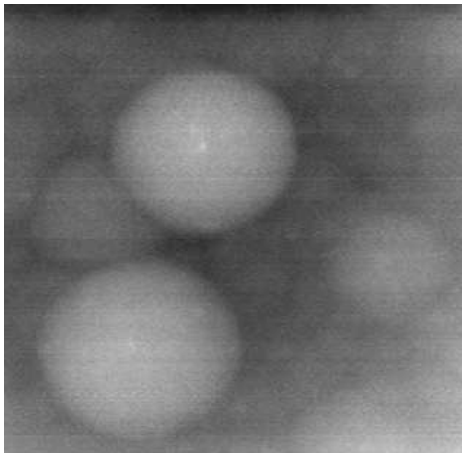

Figure 22 STEM HAADF image of 100-nm Au spheres in 8 μm of water (Source: Joy, workshop participant).

TECHNICAL CHALLENGES

OPPORTUNITIES FOR ELECTRON-SCATTERING INSTRUMENTATION

In the preceding seven challenge areas, workshop participants identified a range of problems that elude characterization with today's instrumentation. Few if any of these challenges can be addressed by existing or planned instruments in the near term. While the seven challenge areas each represent different communities of research, they can all be distilled into two major concepts:

- Achievement of true atomic-resolution characterization (imaging, diffraction, spectroscopy) in *controlled environments of temperature, pressure, or fluidic states*

- High spatial-temporal imaging of dynamic processes of deformation, phase transformations, applied fields, and chemical or multimode processes.

To achieve these goals, a number of individual technical challenges must be addressed; these are outlined below. In some cases these capabilities do not represent entire instruments, but rather what might be considered ancillary developments. This is intentional, since these technological developments can be transferred to the wider community for greater near-term impact.

NEW RESOURCES AND FUNCTIONALITY REQUIRED

As detailed in previous sections, to conduct quantitative observations on changes in the microstructural and microchemical evolution in materials of interest today, a concerted effort in rethinking both the methodology and the technology currently in use for electron beam characterization is needed. Table 2 (from Executive Summary; repeated on following page for convenience) outlines key capabilities and functionalities required to accomplish the scientific challenges enumerated in the preceding sections. These functionalities are grouped within related areas that have common characteristics and, in addition, are prioritized (A = critical; B = high; C = important) relative to their roles in addressing the various scientific challenges.

Each of these six functionalities is addressed below. The requirements for a desired system are documented, and the current state-of–the-art level for commercially available tools is indicated. Note that a number of these challenges/requirements are extreme and may not be readily achievable. These requirements are not simply minor improvements (i.e., factors of 2–3); rather, they require substantial developments, years of work, and a significant financial investment. Also, note that this is not a roadmap on how to achieve these goals, but simply the first step in the process of devising the appropriate path forward. Further community discussion and involvement are required to identify specific pathways.

Table 2 Functionality Required to Address Challenges in Table 1

Functionality Required	Priority
1. In-situ environments permitting observation of processes under conditions that replicate real-world/real-time conditions (temperature, pressure, atmosphere, EM fields, fluids) with minimal loss of image and/or spectral resolution	A
2. Detectors that enhance by more than an order of magnitude the temporal, spatial, and/or collection efficiency of existing technologies for electrons, photons, and/or X-rays	A
3. Higher temporal resolution instruments for dynamic studies with a continuous range of operating conditions from microseconds to femtoseconds	A
4. Sources having higher brightness, temporal resolution, and polarization	B
5. Electron-optical configurations designed to study complex interactions of nanoscale objects under multiple excitation processes (photons, fields, ….)	B
6. Virtualized instruments that are operating in connection with experimental tools, allowing real-time data quantitative analysis or simulation, and community software tools for routine and robust data analysis	C

1. Environmental Instruments: Nature Abhors a Vacuum

Without exception, in-situ instruments were identified as the most important area requiring complete beamline developments. Although efforts in this direction have been under way for some time, combining that ongoing work with aberration-correction technology will have the most impact in the near term. It will not be sufficient to simply attempt to build in-situ stages for ultra-high resolution instruments to achieve this goal. A redesign of the lens area is required — one that incorporates advances in aberration technology and dramatically increases the space for in-situ work.

Technical Objective 1	
Build a suite of dedicated instruments, each of which specializes in a different in-situ environmental geometry, to quantitatively study materials ranging from subnanometer to atomic resolution. The instruments should also have the simultaneous ability to accommodate microanalytical (XEDS/EELS) facilities to characterize the elemental/chemical changes that occur.	
Goals	***Current State of the Art***
Gaseous Environment *Resolution 0.1 nm* *Pressure up to 320 torr* *Temperature to 800°C* *Fluidic Environment* *Resolution <1 nm* *Fully immersed materials in flowing liquid* *Temperature to 200°C* *E/M Field Environment* *Resolution <0.5 nm* *In-plane B fields: 0–500 gauss & zero field out of plane* *In-plane E fields: 0–1 kV/mm & zero field out of plane*	*Gaseous Environment* *Resolution ~ 0.2 nm* *Pressure ~ 5 torr* *Temperature ~800°C* *Fluidic Environment* *Resolution 100 nm* *Static fluid ~ 8 µm of water* *Temperature ambient* *EM Field Environment* *Resolution ~20 nm* *In-plane B fields: ~100 gauss* *In-plane E fields: not implemented*

2. Detectors: Count Every Electron and Make Every Electron Count

Single-electron detectors have been a part of electron beam instruments for more than 30 years, and all modern tools can be easily equipped with this technology. In the last decade, the trend has been to augment these detectors using CCD/CMOS array technology to remove the time-consuming steps involving film. While these array detectors have been adequate for a number of experiments, they still have a number of shortcomings, mainly associated with saturation, noise, limited field of view, and temporal resolution. To significantly improve on all areas of electron imaging, a significant and comprehensive effort must be directed to improving this single area. Next to electron imaging, the detection and analysis of characteristic X-rays in the analytical SEM/TEM/STEM instrument is the most successful and also the second most deployed technology in electron-column instruments. However, this technology has received little attention with respect to improving its analytical sensitivity. Most recent developmental work has concentrated upon improving either spectral resolution and/or processing speed through the use of superconducting materials or silicon drift technology. Although these improvements have been useful, they fail to address the issue that more than 90% of the X-ray signal produced by the electron–solid interaction is simply not utilized. Resolving this problem is critical to studies of beam-sensitive materials or time-resolved experiments, which are becoming increasingly important to the nanoscience community. New designs of X-ray detectors and/or detector arrays, as well as associated changes to the geometry of the electron microscope, are acutely needed. This challenge involves more than simply reengineering the detector itself; it requires new designs of aberration-corrected lenses. These instruments will necessarily not operate at the

highest possible image resolution; instead, they will operate at the highest possible analytical sensitivity and thus significantly complement the efforts in ultra-high-resolution imaging, as represented by the TEAM project goals.

Technical Objective 2	
Develop new generation of electron and X-ray detector systems for use in next-generation analytical electron microscopes.	
Goals	***Current State of the Art***
Electron Detectors: – *4000 x 4000 pixel array detectors, which are radiation hardened to 400 kV* – *24-bit dynamic range* – *< 10 electrons/pixel noise* – *Readout speed of ~ 1Gpixel/sec.* *X-ray Energy Dispersive Detectors Type I:* – *Solid Angle 3 sr* – *Energy Resolution < 120 eV (parallel detection)* – *Throughput 200,000-400,000 cps* – *LN_2 free* *X-ray Energy Dispersive Detectors Type II:* – *Solid Angle ~ 0.5 sr* – *Energy Resolution < 10 eV (parallel detection)* – *Throughput 10 kcps* – *No Liquid Helium Cryostat*	*Electron Detectors:* – *4000 x 4000 pixel array detectors* – *16-bit dynamic range* – *30 electrons/pixel noise* – *Readout speed of ~ 10Mpixel/sec.* *X-ray Energy Dispersive Detectors Type I:* – *Solid Angle 0.5 sr* – *Energy Resolution 140 eV (parallel detection)* – *Throughput 500,000 cps* – *LN2 free* *X-ray Energy Dispersive Detectors Type II:* – *Solid Angle 0.05 sr* – *Energy Resolution 20 eV (parallel detection)* – *Throughput < 1,000 cps* – *Requires Liquid Helium Cryostat*

3. Dynamic Experiments: Time-Resolved and Time-Sliced Instruments

While in-situ instruments were rated the highest priority of the electron beam systems discussed during the workshop, they were followed closely by instruments capable of high temporal resolution and, by extension, environmental instruments that merged both capabilities. There was considerable discussion about the time scales required, which varied with the specific process of interest. At the highest speeds (~ femtoseconds), shock-wave phenomena and structural phase transitions were of primary interest, while at more moderate temporal scales (~ micro- to nanoseconds), EM switching and mechanical deformation dominated the discussion. Both of these are amenable to operation in vacuum and would be early beneficiaries of systems developed for dynamic studies. All dynamic instruments discussed were sufficiently complex that dedicated resources will be required to house and operate them, and thus they likely will be most suitable as user facilities, rather than as individual user tools. The technology required for femtosecond-class instruments is substantially different and more complex than that for a nanosecond-class instrument, and there is a clear transition in the technology between instruments configured for femtosecond response and those in the nano- to picosecond range. The femtosecond regime will likely involve the development of million-volt accelerators and beamlines. Observations of chemical reactions involving gaseous or fluidic environments will also benefit directly from temporal studies; however, these have time scales that can cover the

range from seconds to nanoseconds. In addition to single-shot-type experiments, time-sliced (synchronized) systems should also be pursued to study repetitive processes, such as rapidly oscillating in-plane magnetic fields.

Technical Objective 3	
Build a suite of dynamic instruments covering the three ranges of spatial-temporal resolution.	
Goals	***Current State of the Art***
• *0.1-nm image resolution at 1-μs temporal resolution* • *1.0-nm image resolution at 10-ps temporal resolution* • *100-nm image resolution at 10-fs temporal resolution*	• *0.1-nm image resolution at 100-μs temporal resolution* • *15-nm image resolution at 10-ns temporal resolution*

4. New Electron Sources

Robust and versatile electron sources that improve upon existing technology need to be developed and experimental protocols established for the optimal use and operation of the sources for dynamic studies. Three types of sources dominated the discussion: DC photocathode-pulsed sources, RF photocathode cavities (both of which are applicable to dynamic/time-resolved instruments), and polarized electron sources, which would benefit the magnetic structures community. The DC photocathode sources would be of the highest priority and could also be used to create spin-polarized sources for application in TEM/STEM.

Technical Objective 4	
Develop a robust laser-assisted pulsed photocathode source.	
Goals	***Current State of the Art***
• *Emittance ~0.1 nm rad* • *Electrons/pulse ~10^{8}–10^{12}* • *Pulse width 1 ns–100 fs* • *Energy spread 10^{-5}* • *Spin Polarized*	• *Electrons/pulse ~10^{6} width 10 ns* • *Energy spread 10^{-5}*

5. Multimode Excitation: New Approaches and New Opportunities

Photonics is a rapidly growing field in the nanomaterials area. A major effort should be directed toward configuring an electron-optical beamline that integrates high-resolution analytical electron microscopy with photon-induced phenomena using precisely controlled UV, visible, and IR light sources as well as high-collection-efficiency detectors. This will require efforts similar to the improvements in specimen environment and the objective lens region that are likely needed for improving X-ray detection technology. A new opportunity exists here to explore electron-photon interactions at the subnanometer spatial resolution of the electron microscope. Ideally, this system would also be compatible with Objectives 1 and 2.

Technical Objective 5	
Develop an electron-optical beamline specifically dedicated to combined high-resolution photonics and electron spectroscopy.	
Goals	***Current State of the Art***
• *Electron Probes $\leq$ 0.1 nm* • *Electron Spectroscopic Resolution < 100 meV* • *Multiwavelength (UV, Vis, IR) Optical Probes/Pumps with:* – *optical spatial resolution $\leq$ 0.5 μm* – *scanning probe capable* – *temporal resolution of optical probe ~ 1 ns* – *photon collection solid angles 2-3 sr*	• *does not exist*

6. Virtualization and Community Software

A long-term software resource needs to be developed to provide validated software tools for simulations and analysis for the entire range of experimental methodologies. This development will present tremendous opportunities for quantitative, real-time crystallography on the nanoscale. This resource needs both practicing experimentalists and professional software developers to create, distribute, and maintain a platform-independent repository for the community. In addition, the new capabilities that will be afforded by the preceding developments will create the need to devise new data acquisition, storage, and analysis methods for handling the large influx of data. Real-time processing and display of results during experimental sessions will become an essential component of any user session.

Technical Objective 6	
Create a permanent institute for developing and maintaining community software.	
Goals	***Current State of the Art***
• *Create and fund a long-term institute*	• *does not exist*

RECOMMENDATIONS

In a one and one half-day workshop, it was not reasonable to attempt to develop a comprehensive roadmap to achieve the technical advances outlined in the previous section. Individual roadmaps to overcome the six technological challenges are a logical next step and should be revisited in a deliberative fashion by a select committee of qualified scientists, ideally including a number of the participants in this workshop. Six technological areas have been identified that support the scientific themes that the attendees put forth as having the potential for significant impact within the next decade. DOE should focus its attention on and devote appropriate resources to these six areas to succeed in revolutionizing the capabilities for electron-scattering-based science.

The prospect for addressing these themes is approaching a critical time. A confluence of new technologies will soon offer the opportunity to create a new suite of electron-optical beamlines dedicated to unique modes of characterization. This instrumentation will not emerge without a consistent effort aimed at its development, and DOE should take the initiative by expanding its role from that of stewardship of electron-beam characterization (user) facilities to one that rekindles innovation. Not only should its user facilities be equipped with the state-of-the-art instrumentation, but they should also be supported to carry out development beyond that in which the commercial sector is willing to invest. The judicious investment of resources in moderate- to high-risk ventures can propel the science conducted in electron beamlines well beyond that associated with simple image resolution. It will set the stage for a new era in subnanometer-scale characterization, which will be an essential contribution to nanoscience initiatives around the country.

APPENDIX A: WORKSHOP AGENDA

Thursday, March 1, 2007

Thursday AM - Welcome and Introductory Session

8:30 *Welcome from DOE-BES*
Pat Dehmer / Pedro Montano / Tof Carim
8:45 *Welcome from Organizers*
Dave Williams, University of Alabama - Huntsville /
Dean Miller, Argonne National Laboratory
9:00 *Scientific Introduction to Workshop*
Manfred Ruehle, MPI-Stuttgart, Germany

Scientific Focus Area I: Functional Materials

9:30 Alain Diebold, Sematech
9:50 General Discussion
10:30 ** Coffee Break **

Scientific Focus Area II: Energy Materials

11:00 John Turner, National Renewable Energy Laboratory
11:20 General Discussion
12:00 ** Lunch Break **

Scientific Focus Area III: Small Particles

1:00 Andrew Bleloch, Daresbury Laboratory, United Kingdom
1:20 General Discussion
2:00 ** Coffee Break, regroup into break-out sessions**

Breakout Sessions on Scientific Focus Areas: Development of Grand Challenges

2:15 **Functional Materials**
Breakout Chairs:
Jim Misewich, Brookhaven National Laboratory
Ramamoorthy Ramesh, University of California - Berkeley
Andreas Schmid, Lawrence Berkeley National Laboratory

2:15 **Energy Materials**
Breakout Chairs:
Kath Smith, Australian Nuclear Science and Technology Org.
Ernie Hall, General Electric Corporate Research & Development
Ian M. Anderson, NIST

2:15 **Small Particles**
Breakout Chairs:
Z.L. Wang, Georgia Institute of Technology
Chris Kiely, Lehigh University
Nestor Zaluzec, Argonne National Laboratory

4:15 ** Coffee Break, reconvene plenary session **

Summaries of Breakout Sessions

4:30 **Functional Materials**
4:50 **Energy Materials**
5:10 **Small Particles**

Charge for This Evening's Discussions and Tomorrow's Sessions

5:30 Dave Williams, University of Alabama - Huntsville /
Dean Miller, Argonne National Laboratory
5:45 ** Adjourn for Evening **

Friday, March 2, 2007

Friday AM - Summary of Yesterday's Discussions, Charge for Breakout Session on Enabling Developments

8:30 *Scientific Grand Challenges and Electron Scattering*
Dave Williams, University of Alabama - Huntsville /
Dean Miller, Argonne National Laboratory

Breakout Sessions on Enabling Developments
Discussion and Refinement of Enabling Developments

9:00 **Cross-Cutting Issues**
Breakout Chairs:
John C.H. Spence, Arizona State University
David C. Joy, University of Tennessee
Andreas Schmid, Lawrence Berkeley National Laboratory

9:00 **Relevant Resolutions: Spatial, Temporal**
Breakout Chairs:
Yimei Zhu, Brookhaven National Laboratory
Geoffrey Campbell, Lawrence Livermore National Laboratory
Ian M. Anderson, NIST

9:00 **Sample Environments**
Frances M. Ross, IBM
Ian S. Anderson, Oak Ridge National Laboratory
Nestor Zaluzec, Argonne National Laboratory

10:30 ** Coffee Break **

Summaries of Breakout Sessions

11:00 **Cross-Cutting Issues**
11:20 **Relevant Resolutions**
11:40 **Sample Environments**
12:00 General Discussion and Wrap-up
12:30 ** Lunch **

**** Workshop Adjourns ****
Executive Session Starts

APPENDIX B: WORKSHOP PARTICIPANTS

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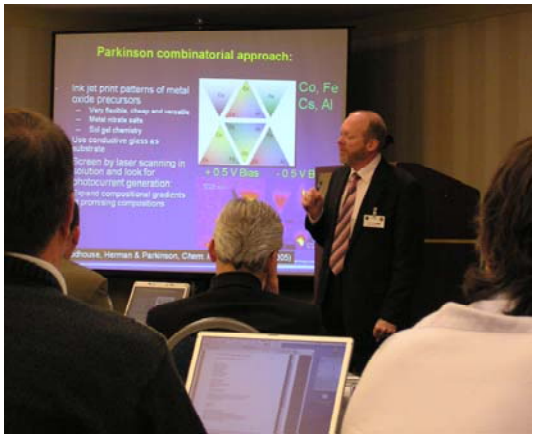
APPENDIX C: DISCUSSION TOPICS CONTRIBUTED BY PARTICIPANTS

PDF copy of presentations available at:
http://www.amc.anl.gov/DoE-ElectronScatteringWorkshop-2007/
Select the link to Documents



Transient Phenomena
Ian S. Anderson - ORNL

Atomic-scale Mechanisms of CO Oxidation Reaction via Heterogeneous Catalysis
Ian M. Anderson - NIST

Spatially Resolved Soft X-ray Emission Spectroscopy to Complement EELS
Phil Batson - IBM

Atomic Level Dynamic Studies
Phil Batson - IBM

Count Every Electron & Make Every Electron Count
Andrew Bleloch - Daresbury

Characterising nano-particles with EM: STEM (EELS and EDX), Stability and Brightness
Andrew Bleloch - Daresbury

Observing Assembly Processes in Solution Based Nanosystems
Paul Braun - UIUC

Imaging Atomic Motion on its Natural Timescale
Nigel Browning - U California - Davis

Materials Development for Power Generation Applications
Gracie Burke - Bechtel Bettis

Femtosecond Materials Science in Irreversible Systems: Experiment at the Scale of Simulation
Geoff Campbell - LLNL

Nanoscale Thermal Imaging
John Cumings - U Maryland

Nanoscale Imaging of Antiferromagnetic Domains
John Cumings - U Maryland

Table Top Analysis
Chiara Daraio - Caltech

Needs and Opportunities for Electron Scattering: Perspective of the Nanoelectronics Industry
Alain Diebold - Sematech

Methods for Characterizing Nanoelectronic Materials and Structures
Alain Diebold - Sematech

Chemistry and Structure of Active Sites for Catalysis
Mark Disko - Exxon Mobil

Ultrafast electron microscopy
Murray Gibson - ANL

Relating Nano/Micro Structure and Chemistry to Macro in Complex Eng. Materials
Ernie Hall - GE

Energy Conversion and Transport at the Nanoscale
Bob Hwang - SNL, CINT

Atomic Imaging of Physiologically Viable Biological and Nano-Bio Materials
David Joy - ORNL, CNMS / U Tennessee

The Sensible Alternative to Electrons - Ion Beams for Imaging and Analysis
David Joy - ORNL, CNMS / U Tennessee

Characterization of Supported Metal Catalyst Systems
Chris Kiely - Lehigh U

Characterization of Complex Nanoparticles and Self-Assembled Metamaterials
Chris Kiely - Lehigh U

3D Dynamic Atomic-Resolution Mapping of Nanomaterials and Interfaces
Brian Korgel - U Texas

Atoms and Fields in Solids
Hannes Lichte - Dresden

Atomic Scale Imaging & Micro-Analysis to Facilitate the Continuation of Moore's Law
John Mardinly - Intel

Electrochemcial Interfaces and Imaging of Nanoparticles
Nenad Markovic - ANL

Dynamical imaging of vortex-defect interactions in superconductors
Dean Miller - ANL

Wet Cell TEM: In-situ Studies in a Liquid Environment
Andy Minor - LBNL

Emergence of Carbon Nanotube Based Device Structures
Jim Misewich - BNL

Imaging Phonons at the Nanoscale
David Muller - Cornell U

Detection, Identification and Quantification of Soft Nanobio Material in Tissue
Anil Patri - NCI / NCL

Fundamental Quantum Mechanical Behavior of Ferroic Nanostructures
Amanda Petford-Long - ANL

Coupling/Decoupling Phenomena
Ramamoorthy Ramesh - U California - Berkeley

Control and Quantification of Thermodynamic Variables for In Situ TEM Studies
Frances Ross - IBM

Integration of In Situ TEM Studies with Advanced Imaging Techniques
Frances Ross - IBM

Future Science Needs and Opportunities for Electron Scattering: Introductory Remarks
Manfred Rühle - MPI Stuttgart

Microscopy under ambient conditions
Miquel Salmeron - LBNL, MF

Magnetism/Spin Imaging at High-Resolution
Andreas Schmid - LBNL

Characterisation and Design of Materials for Gen III+ & IV Reactor Applications
Kath Smith - ANTSO

Dynamics of Deformation in Crystalline Materials
John Spence - ASU

Solving the Structure of Proteins that Cannot be Crystallized
John Spence - ASU

Automated Nanocrystallography at Atomic Resolution
John Spence - ASU

Paying for Electron Scattering Research
Eric Stach - Purdue U

Physical and Electronic Structure of Nanomaterials Susceptible to Radiation Damage
Stephen Streiffer - ANL, CNM

3D Arrangement of Superconducting Vortices
Akira Tonomura - Hitachi

The Time-Frequency Domain
Mike Treacy - ASU

Energy Materials: Meeting Future Energy Challenges for Sustainable Energy
John Turner - NREL

Towards Functional Low Dimensional Materials
Maria Varela - ORNL

Spectroscopy with Sub-Ångström Beams
Maria Varela - ORNL

Surface Atomic Structures of Nanoparticles and Nanowires
ZL Wang - Georgia Tech

In-situ Nucleation and Growth of Nanostructures: Thermodynamics vs Kinetics
ZL Wang - Georgia Tech

In-situ Nanomeasurements and Optical Spectroscopy
ZL Wang - Georgia Tech

Combined Compositional and Diffraction Imaging in 3D TEM at the Atomic Level
Dave Williams - U Alabama - Huntsville

Atomic-scale Mechanisms of Oxidation
Judith Yang - U Pittsburgh

Heterogeneous Catalysis
Judith Yang - U Pittsburgh

Partial Oxidation Reactions in Heterogeneous Catalysis
Gerry Zajac - Inovene

Conformal 3D Mapping of Magnetic Field Distributions
Nestor Zaluzec - ANL

Observing orbital electrons and spins
Yimei Zhu - BNL

Understanding aperiodic structure
Yimei Zhu - BNL

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