



EMSL Quarterly Highlights Report
3rd Quarter, Fiscal Year 2008
(April 1, 2008, through June 30, 2008)

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EMSL is a U.S. Department of Energy (DOE) national scientific user facility located at Pacific Northwest National Laboratory (PNNL) in Richland, Washington. EMSL is operated by PNNL for the DOE Office of Biological and Environmental Research. At one location, EMSL offers a comprehensive array of leading-edge resources and expertise.

Access to the instrumentation and expertise is obtained on a peer-reviewed proposal basis. Users are participants on accepted proposals. Staff members work with users to expedite access. The EMSL Quarterly Highlights Report documents research and activities of EMSL staff and users.

Research Highlights

Atmospheric Aerosol Chemistry

Experimental Studies of Heterogeneous Gas-to-Particle Reactions Using Novel Particle-on-Substrate Stagnation Flow Reactor Approach

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A novel experimental method for measuring net gas-to-particle reaction probabilities has been developed and applied to a number of reactions relevant to atmospheric aerosol chemistry. Systematic studies focused on definitive and quantitative characterization of nitric acid uptake of NaCl, sea salt and CaCO₃ particles under a wide range of relative humidity have been reported using this method.

A novel Particle-on-Substrate Stagnation Flow Reactor (PS-SFR) experimental approach has been developed by staff and users of EMSL to study the kinetics of heterogeneous, gas-to-sea salt particle reactions. In this new approach, substrate-deposited particles are exposed to reactive gases, followed by chemical analysis of the particles, using advanced instrumentation in EMSL. The reactor design and flow parameters were guided by computational fluid dynamics performed by team members from the University of Southern California to ensure that the diffusion flux was uniform for all particles undergoing reaction. The experimental protocol and data interpretation were successfully implemented in laboratory studies focused on heterogeneous gas-to-particle reactions relevant the atmospheric chemistry of sea salt and mineral dust. A complementary combination of the reported results with previously published single particle mass spectrometry data was essential to understanding uptake kinetics over a wide range of particle sizes and experimental conditions. The developed experimental approach offers options for multi-instrumental analyses of particle samples and therefore can be applicable to a wide variety of reactions of interest not only for the atmospheric chemistry community but also for the surface science and catalysis communities.

Heterogeneous reactions between nitric acid and aerosol particles, such as sea salt and carbonates present in mineral dust, serve as major sinks for gaseous metric acid and nitrogen oxides, which impact the overall chemical balance of the troposphere. Results from our studies using the PS-SFR approach show that NaCl and CaCO₃ have a similar reactive HNO₃ uptake at RH<40% but exhibits a very different humidity dependence.

The uptake of HNO₃ onto NaCl was found to increase with the decreasing RH and peak around a relative humidity of 55%, and then below the efflorescence relative humidity (~45% RH) the uptake coefficient decreases rapidly (Figure 1). While uptake of HNO₃ onto CaCO₃ was found to increase monotonically with an increase in relative humidity due to hygroscopic growth of the reaction product Ca(NO₃)₂ (Figure 2). As a result, if CaCO₃ and NaCl aerosol particles are present in the same HNO₃ polluted air mass, both heterogeneous reaction channels could occur. They may take place equivalently or competitively, depending on specific conditions. Sea salt and mineral dust particles are the largest components, by mass, of global aerosol burden and contribute substantially to atmospheric chemistry, air quality, and climate change issues.

The developed approach is expected to be applicable to a variety of reactions of interest not only for the atmospheric research community but also for the surface science and catalysis communities. Details of this research have been recently published in the *Journal of Physical Chemistry A*.

Citations

Liu Y, JP Cain, H Wang, and A Laskin. 2007. "Kinetic Study of Heterogeneous Reaction of Deliquesced NaCl Particles with Gaseous HNO₃ Using Particle-on-Substrate Stagnation Flow Reactor Approach." *Journal of Physical Chemistry A* 111(40):10026-10043.

Liu Y, ER Gibson, JP Cain, H Wang, VH Grassian, and A Laskin. 2008. "Kinetics of Heterogeneous Reaction of CaCO₃ Particles with Gaseous HNO₃ over a Wide Range of Humidity." *Journal of Physical Chemistry A* 112(7):1561-1571.

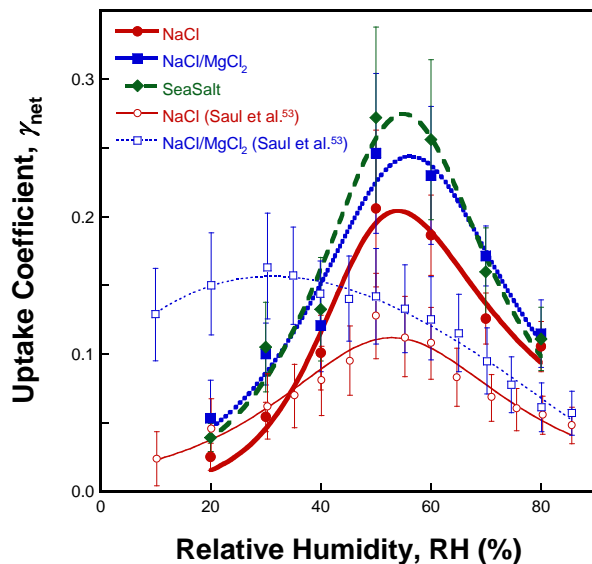


Figure 1. Values of uptake coefficient as a function of relative humidity for HNO₃ reaction with an NaCl, mixture of NaCl/MgCl₂ and sea salt particles (Liu et al, 2007).

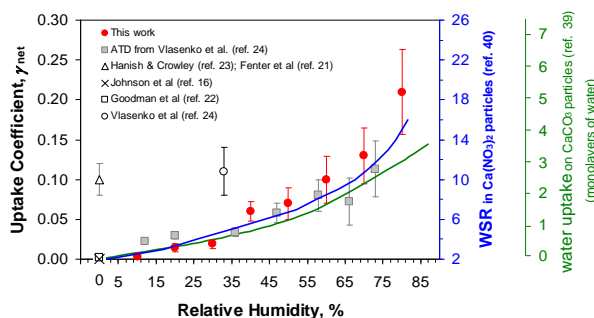


Figure 2. Experimentally determined uptake coefficient as a function of the relative humidity for HNO₃ reaction with CaCO₃ particles (Liu et al. 2008).

Biological Interactions and Dynamics

Submicrometer and Nanoscale Inorganic Particles Exploit the Actin Machinery to be Propelled Along Microvilli into Alveolar Cells

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The explosion in micro- and nanotechnology is expected to increase our exposure to submicrometer and nanoscale particles, but the impact of this exposure on human health is unclear. Since the cellular interactions and pathways of the particles are going to drive cellular response and ultimately the level of toxicity, we have been studying these cellular processes while focusing on well-defined particles and delineating relationships between particle properties and potential toxicity or biocompatibility.

The environmental or occupational exposure to submicrometer and nanoscale materials is expected to increase within the next few years as the result of their increased use in industrial and medical applications. When inhaled, these particles are likely to reach the alveoli, where alveolar type II epithelial cells are found. These cells, which are distinguished by apical microvilli, play critical roles in the function of the alveoli and participate in the immune response to certain particles and pathogens by releasing chemokines. However, the cellular interactions of the particles, which drive the cellular responses, are still unclear. Adverse effects of nanoparticles have been attributed, in part, to the unique properties of materials at the nanoscale. However, little is known about the cellular interactions of individual or small nanoparticle aggregates, mostly because of their tendency to agglomerate under experimental conditions.

Since the cellular interactions and internalization pathways of inhaled particles are going to drive the cellular response and ultimately the impact on

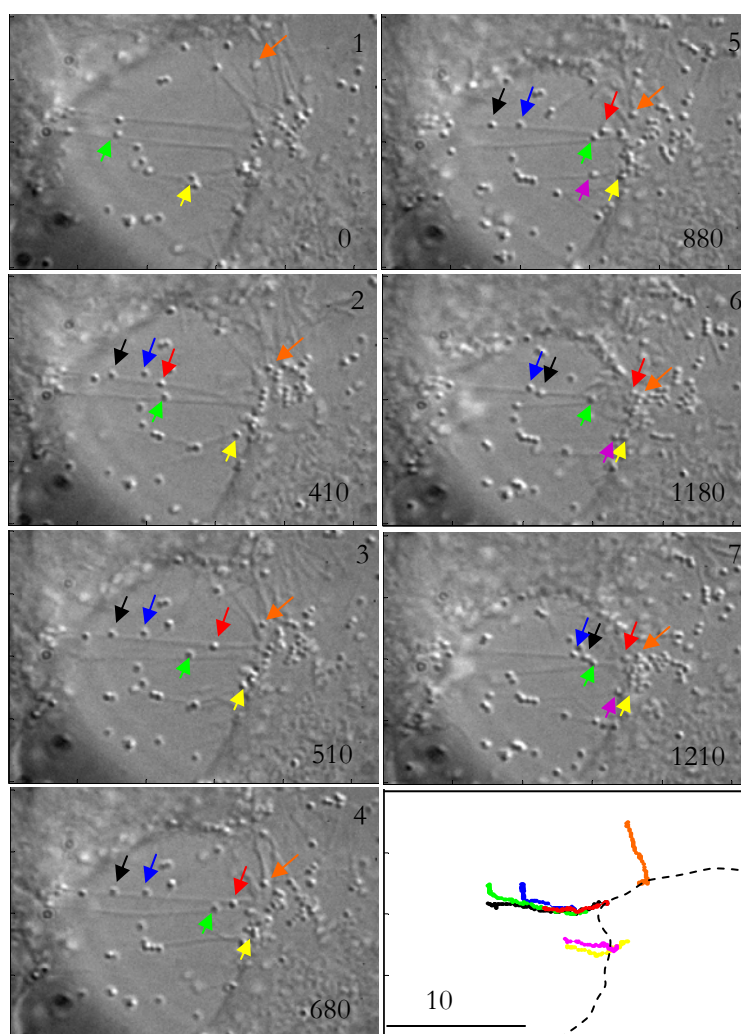


Figure 1. The retrograde motion unravels the coupling of the particles with the intracellular environment across the cell membrane.

the pulmonary system, we investigated the surface-dependent interaction of individual or small aggregates of submicrometer and nanoscale particles, as they are likely to be presented to cells *in vivo*. Using differential interference contrast (DIC) and total internal reflection fluorescence (TIRF) microscopy at 200 times magnification, we find that positively charged 100-nm and 500-nm precipitated amorphous silica particles can travel along microvilli toward the cell body. The retrograde motion unravels the coupling of the particles with the intracellular environment across the cell membrane. Figure 1 demonstrates the retrograde motion of positively charged 500-nm particles, using a time series of DIC images that were acquired at 10-second intervals. Each particle is followed along the sequence of the images with a color-coded arrow that is added when the particle lands on the cell. Particles can dwell in their landing spot before starting to move, or become engaged in the motion immediately after landing. By the end of the series, the particles are found by the cell body where other particles are already accumulated.

Figure 2 demonstrates the retrograde motion of 100-nm particles using single-molecule fluorescence techniques. The images in Figure 2a were selected from a time series that was acquired using TIRF microscopy at 10-second intervals. The fluorescent spot that is indicated by the arrow in the first image is estimated to represent one nanoparticle or a cluster containing two nanoparticles. The estimation is based on the intensity of the fluorescent spot and on the size of the spot, which is near the diffraction limit of the light (3 x 3 pixels). The particle travels along a microvillus that originates from the apical surface of the cell body, as shown in Figure 2b where the trajectory of the nanoparticle is overlaid on the DIC image. Interestingly, the motion pattern of the nanoparticle, although clearly directed toward the cell body, includes both rearward and forward motions, as demonstrated in the trajectory.

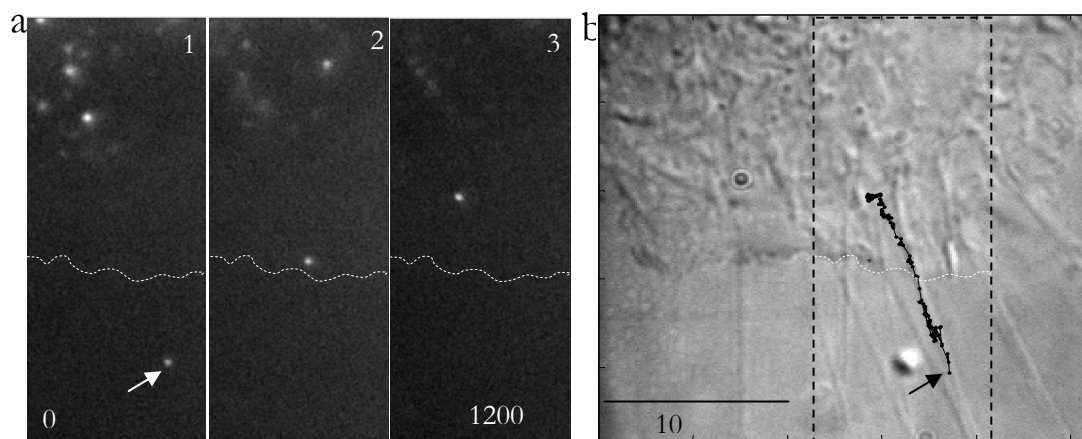


Figure 2. The retrograde motion of 100-nm particles using single-molecule fluorescence techniques.

By studying both negatively and positively charged particles, we found that only the positively charged particles can undergo a retrograde motion. This observation indicates that the motion is dependent on electrostatic interactions between negatively charged molecules in the plasma membrane and the positively charged surface of the particles. We also observed positively charged particles undergoing a retrograde motion in ATP depleted cells, which indicates that the motion is not powered by myosin or other ATP-dependent motor proteins. However, we found that the motion is strongly dependent on the integrity of the actin filaments within the microvilli. Actin filaments at the leading edge of many cells undergo a continuous cycle of assembly at their distal barbed end and disassembly at their proximal end. This treadmilling underlies a process termed actin retrograde flow. By transfecting the cells with fluorescent actin, which allowed us to follow the motion of actin clusters, and by applying drugs that inhibit the flow, we found that the actin treadmilling powers the retrograde motion of the particles, as illustrated in Figure 3.

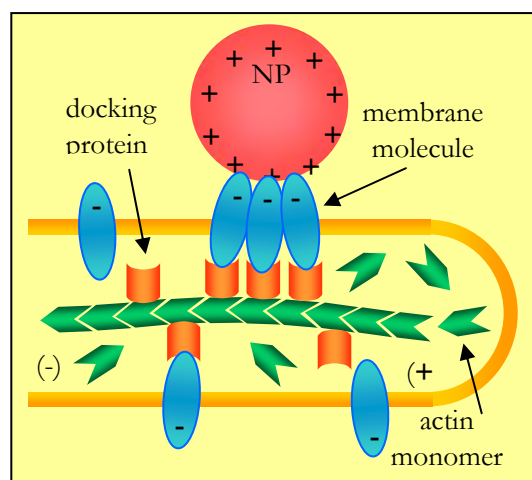


Figure 3. Researchers found that the actin treadmilling powers the retrograde motion of the particles.

Citation

Orr G, DJ Panther, JL Phillips, BJ Tarasevich, A Dohnalkova, D Hu, JG Teeguarden, and JG Pounds. 2007. "Submicrometer and Nanoscale Inorganic Particles Exploit the Actin Machinery to be Propelled along Microvilli-like Structures into Alveolar Cells." *ACS Nano* 1(5):463-475.

Zinc is Focus of Integrated Studies to Understand Metalloprotein Structure and Function

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Many critical biological functions, including DNA repair, depend on proteins with reactive metal centers. Understanding the structure of these proteins at the molecular level gives researchers insight into how those proteins carry out their very important jobs.

Refining molecular theory using experimental data furthers researchers' understanding about the metal environment in structural and reactive sites of proteins, gaining strides in EMSL's focus to predict biological functions from molecular and chemical data.

Predictive models for metalloproteins are gaining accuracy because of integrated research using supercomputing and nuclear magnetic resonance spectrometry capabilities housed at DOE's EMSL. In a series of studies to relate metal-center protein environments to structure and function, a research team from EMSL and Pacific Northwest National Laboratory is using EMSL's NWChem computational chemistry software and NMR spectroscopy to derive a molecular theory that describes the electronic environment of the metal-amino acid motif, zinc coordinated to four cysteines. This motif was once thought to only play a structural role, but is now known to play a reactive role as well, for example, facilitating DNA repair.

In previous experiments, the research team used model proteins containing the zinc-cysteine motif to find a level of theory adequate to predict NMR results (Lipton and Ellis 2007). In the new phase of their studies described here, the team refined their model using a real-world example: zinc-substituted rubredoxin derived from the thermophile, *Pyrococcus furiosus* (Figure 1). Rubredoxins play a role in electron transfer – an important regulatory mechanism in biological systems. In zinc-substituted rubredoxin, the iron center of rubredoxin’s active site is substituted with zinc, serving as a system of study for a zinc-cysteine site with only a structural role. To predict NMR data in this real-world scenario, computational theory requires a combination of quantum mechanics and molecular mechanics. In comparison to the level of computational theory required to describe the model proteins in previous studies, anisotropic shielding must be more heavily account for – in other words, NMR spectra peak characteristics measured at the zinc site are more dependent on the electron densities and the point of view of the observer for rubredoxin. In future studies, similar sites with reactive roles will be compared. This research was reported in the *Journal of the American Chemical Society* (Lipton et al. 2008).

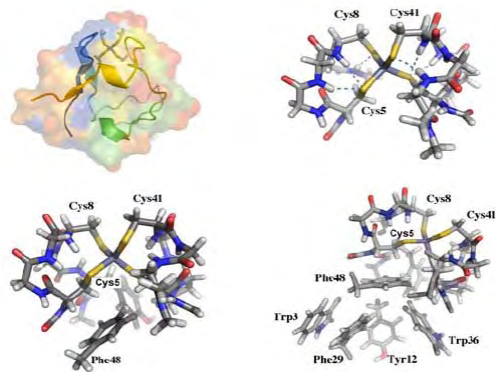


Figure 1. Structure of the zinc- and cysteine-containing region of *Pyrococcus furiosus* rubredoxin determined with different computational chemistry models.

Citations

Lipton AS, and PD Ellis. 2007. “Modeling the Metal Center of Cys₄ Zinc Proteins.” *Journal of the American Chemical Society* 129(29):9192-9200.

Lipton AS, RW Heck, M Valiev, WA de Jong, and PD Ellis. 2008. “A QM/MM Approach to Interpreting ⁶⁷Zn Solid-state NMR Data in Zinc Proteins.” *Journal of the American Chemical Society* 130(19):6224-6230.

Geochemistry/Biogeochemistry and Subsurface Science

None reported during this quarter.

Science of Interfacial Phenomena

Laser and Electrical Current Induced Phase Transformation of In₂Se₃ Semiconductor Thin Film on Si(111)

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Materials with rapid and reversible switching between amorphous and crystalline phases, and which exhibit significant electrical resistivity or optical reflectivity change between these phases, are promising candidates for phase-change non-volatile memory. The

strong change in optical reflectivity during the amorphous-crystalline phase transition is the basis of re-writeable compact disk and digital video disk technology. During the past decade, binary chalcogenide semiconductors such as InSe/GaSe and In₂Se₃ have been investigated as potential phase-change media in proposed data storage and memory devices. This research investigates the phase-change mechanisms of In₂Se₃ using EMSL's photoemission electron microscope capability. This research will be highlighted in a journal article published this summer in Applied Physics A.

The electrical resistivity of In₂Se₃ increases by a factor of 10⁵ from the crystalline to the amorphous state. However, the structural details of phase-change in In₂Se₃ films on silicon and the energetic requirements for phase change have not been fully explored. In₂Se₃ exhibits a complex phase system in which various structures with different arrangements of inherent defects can form. This complexity originates from many energetically similar routes by which trivalent and divalent atoms can combine to satisfy their bonding requirements and leads to several crystalline phases with the same In₂Se₃ stoichiometry.

This research analyzes the crystallization and amorphization of In₂Se₃ thin films on Si(111) (~ 30 nm thick) via resistive heating and laser annealing, respectively. The initially amorphous films were crystallized using resistive heating (time-scale of several seconds), while a 150-micron-diameter spot was re-amorphized using nanosecond laser annealing. The film morphology and conductivity were probed with scanning tunneling microscopy and photoelectron emission microscopy (PEEM), the crystallinity was probed with x-ray diffraction and low-energy electron diffraction, and the stoichiometry with Rutherford back-scattering spectroscopy. The stoichiometry, morphology, and crystal structure of the crystallized In₂Se₃ film and its orientation with respect to the substrate are determined.

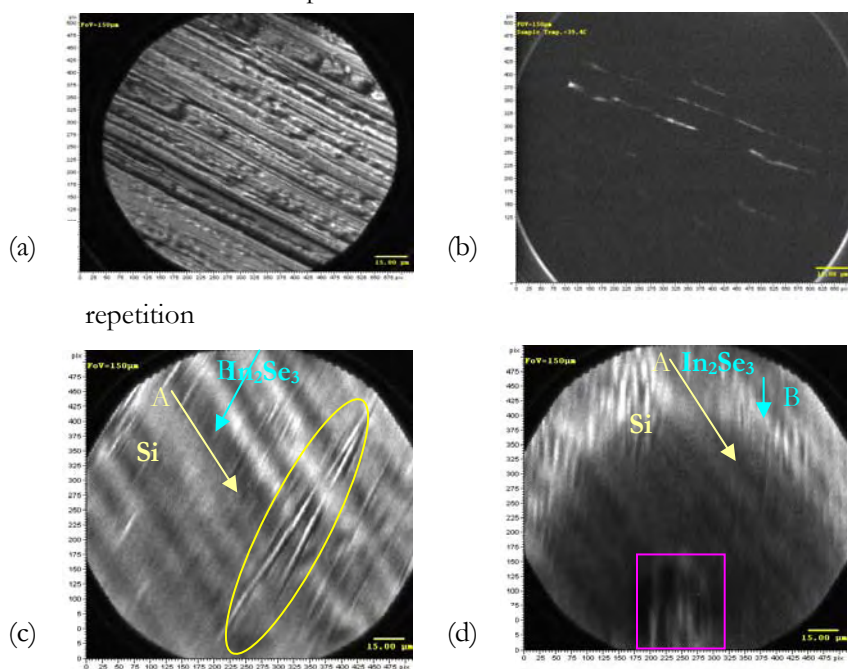


Figure 1. PEEM images (field of view 150 μm , scale bar 30 μm) for (a) clean Si(111); (b) amorphous In₂Se₃ film on Si(111); (c) annealed In₂Se₃/Si(111); (d) after irradiation with 266-nm photon pulse. Images presented here are acquired with mercury lamp illumination ($h\nu = 5.1$ eV).

The EMSL PEEM was equipped with both Hg ($h\nu = 5.1$ eV) and D₂ ($h\nu = 6.0$ eV) sources for imaging a 150- μm -diameter region of the sample. An Nd:YAG laser ($\lambda = 266$ nm, $h\nu = 4.7$ eV, FWHM pulse width 20 ns, spot diameter 100 μm , 0.1 mJ/pulse at 1 Hz rate) was interfaced to the PEEM and used to amorphize the crystalline film. The laser is introduced through an ultraviolet-grade-fused silica window to the PEEM objective chamber holding the sample.

While a slow anneal below the melting temperature can lead to crystallization of an amorphous film, returning to the

amorphous state requires rapid heating and cooling to quench in the disordered state. This was accomplished with pulsed laser annealing. The sample was monitored with the PEEM, which distinguishes structures on the surface through a combination of their work function, electrical conductivity, and

density of states near the Fermi level.

Figure 1(a) shows a PEEM image of a clean Si(111) substrate after being argon-sputtered and then annealed around 850°C. An amorphous In₂Se₃/Si(111) film deposited is shown in Figure 1(b). The room-temperature-deposited In₂Se₃ film presents a completely dark PEEM image when using either the mercury lamp (5.1 eV) or D₂ lamp (6.0 eV), except for defect lines running through the center of the image.

A PEEM image was obtained of the same film before [Figure 1(c)] and after [Figure 1(d)] laser annealing. Similar results were obtained with both mercury and D₂ illumination, although only the mercury results are shown. Comparison to silicon substrates without In₂Se₃ films [Figure 1(a)] indicates that the wider stripe structure running from upper left to lower right arises from the underlying silicon terrace structure (yellow arrows), while the narrower lines (blue arrows) correspond to the texture of the In₂Se₃ films. Two crossed lines marked in the oval are defects on the surface.

The 266-nm laser was used to anneal a spot on the sample approximately 150 microns in diameter near the place where the image in Figure 1(c) was taken. Single pulses of 0.1-mJ and 20-ns duration were measured at the laser head. Subsequent aperture-reduction and focusing culminated in a final pulse fluence of < 50 mJ/cm². The resulting annealed region is shown in Figure 1(d), where a dark circular region may be observed surrounded by features characteristic of the crystalline In₂Se₃ film. The darker region still shows (though with less contrast) the structure characteristic of the underlying silicon substrate, with In₂Se₃ features less distinct.

The contrast between the crystalline and amorphous regions in the PEEM could arise from differences in work function, in densities of states near the Fermi level, or in film conductivity. The work function of crystalline In₂Se₃ is 4.35 eV, so both mercury (5.1 eV) and D₂ (6.0 eV) illumination should result in electron emission. Our photoemission measurements on a 1-nm-thick film show an In 4d core level shift of ~ 0.7 eV to higher binding energy (relative to the Fermi energy) from the amorphous to the annealed phase, while the silicon 2p shifts by only 0.1 eV in the same direction. If the In shift were completely due to a change in work function, then the mercury radiation would be close to threshold for photoemission, but there should still be significant emission with D₂ radiation. However, we find no emission with either source for the as-deposited film except at large-scale defects [Figure 1(b)]. It is thus likely that photoexcited electrons become trapped in the highly resistive amorphous material and cannot travel to the surface for emission into vacuum.

The control of material phase (amorphous, or one of several possible crystalline or polycrystalline states) is essential to the properties of modern devices. The difference in properties associated with a phase change may be exploited for device operations, as in DVDs where the change in optical reflectivity between crystalline and amorphous states allows media rendition. Driven by the need for a new paradigm to continue the relentless increase in both density and speed that has characterized developments in computer memory for four decades, one promising avenue for non-volatile memory is phase-change non-volatile memory, for which chalcogenides are prime candidates.

Amorphous-crystalline phase transitions can be achieved by applying voltage pulses with different amplitudes and durations in the range of tenths of nanoseconds. In our study, we have shown that rapid, selective, and local crystal-amorphous transformation can be realized using pulsed, ultraviolet nanosecond lasers at low fluences. This is a necessary step in the development of high-density/high-speed chalcogenides-based optical phase-change non-volatile memory.

Hidden Ferromagnetic Secondary Phases in Cobalt-Doped ZnO Epitaxial Thin Films

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Spintronics has the potential to revolutionize electronic devices by effectively using the spin degree of freedom. However, developing the required materials necessary for room temperature operation presents a serious materials physics challenge. Investigation of potential dilute magnetic semiconductor (DMS) materials utilizing semiconducting oxide hosts was motivated by both theoretical and experimental findings of ferromagnetism at room temperature in doped oxides.

Despite the enormous body of research that has followed, no unambiguous demonstration of carrier-mediated ferromagnetism has been made. Disparate and irreproducible experimental results have led to serious doubts as to whether the observed ferromagnetism is intrinsic to the doped oxide system or due to extrinsic effects such as contamination or phase impurity. As one example, the reported magnetization values for Co:ZnO range over two orders of magnitude (paramagnetic to $<0.05 \mu_B/\text{Co}$ to $>6 \mu_B/\text{Co}$). Recently, our group has shown that structurally well-defined cobalt-doped ZnO is not intrinsically ferromagnetic, either in the semi-insulating state or when electronically doped *n*-type.

Weak ferromagnetism in Co:ZnO ($0.1 - 0.3 \mu_B/\text{Co}$) has been induced by annealing in zinc vapor to diffuse interstitial zinc (Zn_i) into the Co:ZnO lattice. The proposed model for ferromagnetism in the presence of Zn_i involves specific defect/donor formation which facilitates electron-mediated cobalt spin alignment.

In collaboration with researchers from the Advanced Photon Source at Argonne National Laboratory, researchers at Pacific Northwest National Laboratory have further explored the origin of ferromagnetism in epitaxial $\text{Zn}_i\text{:Co:ZnO}$ thin films which have undergone a similar zinc vapor treatment. High-quality epitaxial $\text{Co}_x\text{Zn}_{1-x}\text{O}$ thin films were deposited in EMSL by pulsed laser deposition on single crystal sapphire (Al_2O_3) substrates. Treatment in zinc vapor was accomplished by sealing the films in an evacuated quartz tube containing zinc metal, then heating to 600°C for 5 hours.

After the zinc vapor treatment, the films were found to be ferromagnetic at room temperature ($\sim 0.05 \mu_B/\text{Co}$), a necessary condition for a spintronic material.

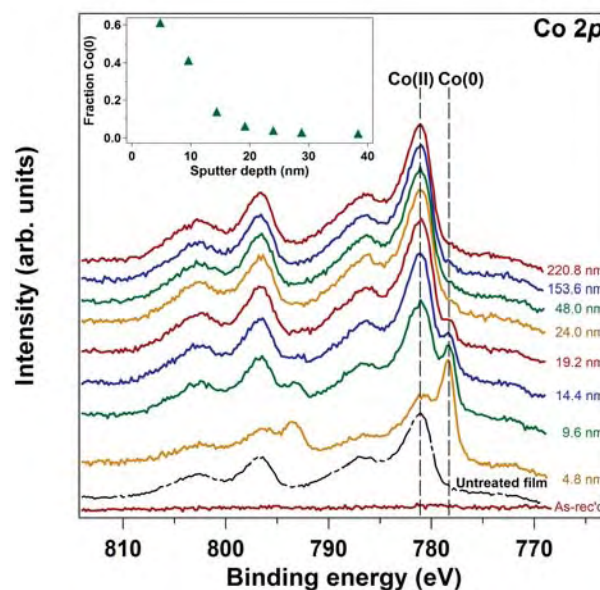


Figure 1. X-ray photoelectron spectroscopy depth profiles of 310 nm $a\text{-Co}_{0.1}\text{Zn}_{0.9}\text{O}$ after zinc treatment. For comparison, the cobalt 2p spectrum of an untreated film after one sputter cycle is shown (dash-dot line). Inset: fraction of cobalt present as Co(0) as a function of depth in $\text{Zn}_i\text{:Co:ZnO}$, as determined by fitting the x-ray photoelectron spectroscopy cobalt 2p spectra.

Initial materials characterization by grazing-incidence x-ray diffraction and x-ray absorption near edge spectroscopy indicated that no phase segregation or cobalt reduction occurred, implying the ferromagnetism is intrinsic to Zn_n:Co:ZnO (Figure 1). However, when incorporating cobalt as a dopant, there is *always* the possibility of ferromagnetic secondary phase formation which can result in a weak spurious ferromagnetic signal that may be mistaken for intrinsic ferromagnetism in the doped oxide. The very weak ferromagnetism observed after zinc treatment could result if only 3 percent of the cobalt dopants formed cobalt metal precipitates; secondary phase formation at this level is below the detection limit of these sophisticated material characterization techniques.

Thus, a more careful analysis utilizing x-ray photoelectron spectroscopy at EMSL and x-ray absorption at the Advanced Photon Source was undertaken to more thoroughly investigate the possibility of cobalt metal secondary phase formation. High resolution x-ray photoelectron spectroscopy depth profiling revealed metallic cobalt in the near-surface region of the Zn_n:Co:ZnO film; further analysis by x-ray absorption identified the ferromagnetic secondary phase as intermetallic CoZn, which has never previously been reported in Co:ZnO. From these results, the observed ferromagnetism was shown to arise from this secondary phase, not from intrinsic ferromagnetism in Zn_n:Co:ZnO. This work emphasizes the vigilance required in materials characterization before intrinsic ferromagnetism can be definitively attributed to the substitutionally doped oxide phase.

This work was published in *Physical Review B* as a Rapid Communication and was subsequently selected as a research highlight by *Nature Materials* [7(7):517].

Citations:

Kaspar TC, T Droubay, SM Heald, MH Engelhard, P Nachimuthu, and SA Chambers. 2008. "Hidden Ferromagnetic Secondary Phases in Cobalt-Doped ZnO Epitaxial Thin Films." *Physical Review B* 77(20):201303.

A Fast Analysis Technique to Evaluate Scintillation Response

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Demands for national security, medical physics, and high-energy nuclear physics applications have prompted research efforts for both improved performance of materials for radiation detection and accelerated materials discover (van Eijk 2003). Existing detector materials do not meet the increasing requirements of nuclear nonproliferation and homeland security applications. Next-generation radiation detector materials with excellent energy resolution at room temperature are needed. Both accelerated materials discovery and efficient techniques that can investigate material properties relevant to detector performance are required.

For gamma ray (γ -ray) detection, a relatively large high-quality crystal is needed for complete absorption of γ -ray energies of interests. New materials discovery has been limited due to the difficulties inherent to large crystal growth; whereas high-quality thin films of candidate materials can be readily produced by various modern deposition techniques. Charged particles, such as He⁺, can easily deposit all their energy within a few tens of micrometers, and the corresponding scintillation response can be used to characterize material properties relevant to detector performance. In the current study, a fast screen technique, applicable to thin films or small crystals, is demonstrated to provide the scintillation response of the materials, where energetic

ions are used instead of gamma rays. Benchmark materials of bismuth germanate (BGO, $\text{Bi}_4\text{Ge}_3\text{O}_{12}$) and europium-doped calcium fluoride ($\text{CaF}_2:\text{Eu}$) crystals are chosen to demonstrate the ion approach.

Experimental Procedures

The scintillation response of materials to He^+ was measured using a time-of-flight (TOF) setup. He^+ ions with energy of 3.5 MeV were produced using a forward scatter method, as shown in Figure 1. Monogenic particles of helium were produced by an NEC tandem accelerator and forward scattered at 45 degrees to the primary beam direction into the TOF telescope by a bulk gold target. Using the forward scatter method, energetic He^+ particles were produced over a continuous range of energies from a few tens of keV to a few MeV, so the scintillation response could be investigated over a continuous energy range.

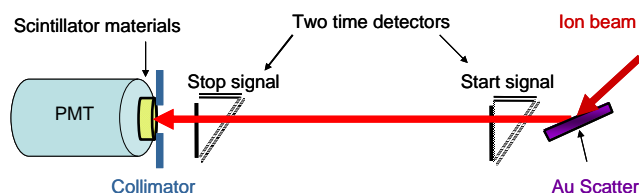


Figure 1. Schematic drawing of the TOF-scintillator-PMT setup for the scintillation measurement, where BGO or $\text{CaF}_2:\text{Eu}$ is mounted between the second time detector and the PMT.

Results and Discussion

Energy Resolution

To demonstrate that the current approach that can be used as a fast screening technique, the scintillation response of both BGO and $\text{CaF}_2:\text{Eu}$ was examined, and the results are shown in Figure 2. With superior energy resolution and fast response of the TOF telescope, the energy of individual particles before impinging on the scintillating crystal were determined with a high counting rate. In about 30 minutes, more than 1 million particles were detected by both the $\text{CaF}_2:\text{Eu}$ crystal and the TOF telescope in a coincident mode, which allows quantitative analysis of material performance over a continuous energy range in a relatively short time.

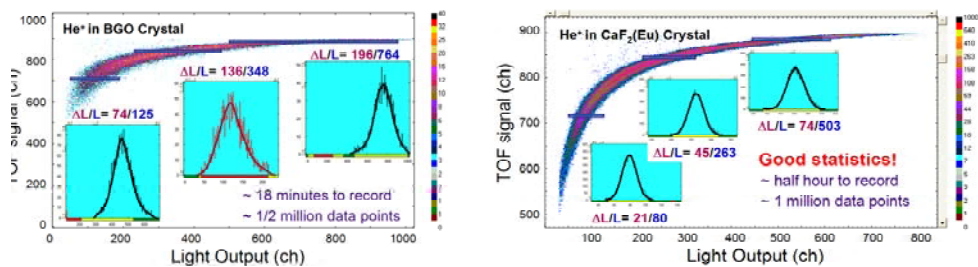


Figure 2. TOF versus light output of BGO (left) and $\text{CaF}_2:\text{Eu}$ (right) to He^+ particles. The insets are the light output profile of the particle at TOF=715, 840 and 885, respectively. The light intensity is governed by the peak position L and the energy resolution can be determined by $\Delta L/L$ as shown by the three insets.

The measured energy resolution in the current study is defined as the full width at half maximum (FWHM) of the peak normalized to its energy ($\Delta L/L$). Fast determination of energy resolution of scintillation response can be obtained by online analysis, as shown by the three examples with corresponding $\Delta L/L$ values in Table 1 and Figure 2. Compared with the BGO crystal, the $\text{CaF}_2:\text{Eu}$ crystal indicates a much better energy resolution, as demonstrated by the examples at three energies (different TOF).

TABLE I
FAST ESTIMATION OF ENERGY RESOLUTION ($\Delta L/L$) OF SCINTILLATION RESPONSE

TOF (ch)	BGO	$\text{CaF}_2:\text{Eu}$
715	59%	26%
840	39%	17%
885	26%	15%

Light Yield

Absolute light yield is one of the critical properties when evaluating a scintillation material. The scintillator light yield in this study is given by the pulse height (related to the number of photons) measured due to the total energy deposition of the impinging particles. The scintillation response of the two crystals was measured over the energy range from about 100 keV to approximately 3400 keV using the current technique. As shown in Figure 3, much higher light yield is observed for $\text{CaF}_2:\text{Eu}$, as compared with BGO. The relative ratio is in good agreements with the literature value from gamma ray measurements, where the absolute light yield is 8,200 and 24,000 photons/MeV for BGO and $\text{CaF}_2:\text{Eu}$, respectively (Knoll 2000; Holl et al. 1988).

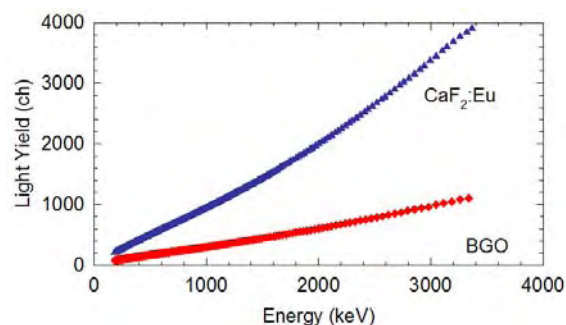


Figure 3. Light yield (L) as a function of particle energy (E) for $\text{CaF}_2:\text{Eu}$ and BGO from a similar experimental setup.

Conclusion

For fast screening purposes, the candidates of radiation detector materials can be simply investigated using readily available energetic ions, such as hydrogen or helium ions. The measured light yield and energy resolution observed in the candidate scintillation materials can be compared with the results from benchmarked detector materials. This approach can be applied as a fast analysis technique to assist current efforts on the discovery of new radiation detection materials. The primary assumption is that thin-film materials or small crystals, whose energy resolution to alphas is poor, are unlikely candidates for gamma detectors, while materials that demonstrate good detector response are candidate materials for further investigation, including large crystal growth.

Furthermore, the use of charged particles to deposit energy provides additional control and separation of mechanisms related to photon response and transport properties. This work demonstrates a possible pathway to achieve fundamental understanding of charged particle response and energy resolution, which may provide insight into the different mechanisms that govern the scintillation processes and the origins of light yield nonlinearity in different materials.

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Microstructures of ZnO Films Deposited on (0001) and r-cut α -Al₂O₃ Using Metal Organic Chemical Vapor Deposition

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ZnO is a wide-bandgap semiconductor material with wide application in the field of optoelectronics, spintronics, piezoelectric transducers, and ultraviolet optoelectronics (Fan and Liu 2005). Considerable research effort has been made for modifying the properties of the ZnO through tailoring of the structure of the material, typically such as doping, grown ZnO into different dimensional structures (dots, thin film, and bulk materials). One of most useful forms of ZnO is the thin film. The key challenge for growing ZnO into a thin film is the control of defect structure in the film, because defects influence the optical and electrical properties of the film. Selection of the substrate and the control of the defect across the interface between the substrate and the film play an important role on the quality of the grown film. This research addresses the defect structure of the ZnO thin film grown on a sapphire substrate.

ZnO grown on (0001) sapphire will generally be oriented such that α -Al₂O₃ (0001)//ZnO(0001). Variable in-plane orientation may lead to two domains such that: α -Al₂O₃ [11-20]//ZnO[11-20] and α -Al₂O₃ [11-20]//ZnO[10-10]. The first mode corresponds to the hexagon-on-hexagon growth and the second mode corresponds to a 30-degree in-plane rotation of the ZnO relative to the α -Al₂O₃. Since it is difficult to obtain an ideal sapphire surface with a well-defined surface structure, various rotation domains, such as the 30-degree rotation domains and a recently reported 21.8-degree rotation domain, may coexist. A previous study shows that by using gallium pre-deposition to modify the sapphire (0001) surface, rotated domains can be completely eliminated. Another growth parameter that could be controlled is the selection of the orientation of the substrate. It has been generally realized that ZnO grown on r-cut sapphire possesses a high quality. However, there is no direct comparison of the film quality grown on both r-cut and c-plane oriented sapphire under an identical growth condition.

In this paper, we report a comparison of the structural features of ZnO thin films grown on both r-cut and c-plane sapphire using metal organic chemical vapor deposition (MOCVD) under identical growth conditions (Wang et al. 2008). It has been found that the film grown on r-cut sapphire shows high-quality single crystals. Film grown on the c-plane shows a range of domains, one that corresponds to the classic growth mode. At the same time, a new growth mode was observed following the deposition of ZnO thin film on α -Al₂O₃ (0001). In this new growth mode, α -Al₂O₃ [11-20]//ZnO[10-10], but the (0001) plane of ZnO is tilted relative to the (0001) plane of α -Al₂O₃ such that ZnO(0001) is almost parallel to the α -Al₂O₃ (-1104) plane.

Growth of the film was performed using a three-source EMCORE MOCVD reactor. The precursor preparation was done by dissolving $\text{Zn}(\text{C}_{11}\text{H}_{19}\text{O}_2)_2$ -Bis(2,2,6,6-tetramethyl-3,5-heptanedionato) zinc powder in tetrahydrofuran at a concentration of 0.025 M. During the depositions, the substrates were rotated at 500 rpm and the substrate temperature was varied between 450 °C to 600 °C. The carrier gas pressure during the growth was kept at 0.28 MPa with a zinc precursor flow rate of 100 g/hr. The operating pressure was kept at 10 Torr with a mixed gases of oxygen and argon flows of 500 sccm and 2000 sccm, respectively. Single crystals of α - Al_2O_3 (0001) and r-cut α - Al_2O_3 were used as substrates.

The film grown on r-cut α - Al_2O_3 possesses a single orientation with respect to the substrate. The interface shows some contrast features that are related to the mismatch dislocations. This feature is further revealed by the high-resolution transmission electron microscopy image illustrated in Figure 1. The interface was featured by very high density of misfit dislocations. The dislocation is not evenly distanced along the interface. Rather, it appears that the dislocation is coupled, leading to a pattern of two dislocations forming a pair. The physical reason for this must be studied. Across the interface, on average, every sixth of α - Al_2O_3 (-12-10) plane terminates at the interface. This result is consistent with that when the film grown on the α - Al_2O_3 (0001) plane. However, the dislocation appears to be uniformly distributed when grown on the (0001) direction. Using the α - Al_2O_3 (-12-10) lattice plane space of 2.3794 Å as an internal standard, the ZnO (01-10) lattice plane space was determined to be 2.773 Å. This will lead to a lattice constant for ZnO to be 3.202 Å, which is slightly smaller than the literature data of 3.249 Å.

ZnO films grown by MOCVD on α - Al_2O_3 (0001) using the $\text{Zn}(\text{TMHD})_2$ precursor show granular structures and the grains possess different orientations. Based on electron diffraction and high-resolution transmission electron microscopy imaging, at least two distinct orientations have been identified. One corresponds to the classic 30-degree in-plane rotational domain. The other also includes the 30-degree rotational domain, but, instead of the ZnO (0001) plane being parallel to the (0001) plane of α - Al_2O_3 , the (0001) plane of ZnO is tilted \sim 38-degrees in such a way that the (0001) plane of ZnO is approximately parallel with the (-1104) plane of α - Al_2O_3 . This tilting of the (0001) plane results in a reduction of interface lattice mismatch from \sim 18 percent to \sim 2 percent in one direction. Therefore, the tilted growth mode was driven by minimization of interfacial energy. The film grown on r-cut α - Al_2O_3 showed a single crystalline structure and the interface was featured by a high density of mismatch dislocations.

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Figure 1. High-resolution transmission electron microscopy image showing the interface between α - Al_2O_3 and ZnO with the film grown on r-cut α - Al_2O_3 .

Enhanced Understanding of Titania's Catalytic Mechanism through Computational Modeling

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Using EMSL's computational modeling capabilities, fundamental insight into the properties of titania surfaces is obtained, which is knowledge necessary for understanding the potential use of titania-based catalyst for providing a source of hydrogen fuel and a the potential for aiding in Hanford Site cleanup.

Since the dawn of time, mankind has been driven to obtain both energy and an understanding of where this energy came from, and more importantly how to control it. While early mankind only had fire and little understanding, modern man has a multitude of energy choice with more choices on the horizon. Unfortunately, even though the world's economy is driven by energy, understanding is does not always keep up with these advances, and without understanding we will not be able to make the right choices as a nation or as individuals.

Recently, hydrogen has gained much attention as an environmentally friendly energy medium. Titania (TiO_2) has been the subject of extensive research because of its potential use as a catalyst for the production of hydrogen via water splitting. For example, experimentalist have already shown that trimethylacetic acid can be decomposed into isobutene and carbon dioxide on titania, but the theoretical models are not advanced enough to explain the fundamental interactions. In the dynamic realm of condensed phase chemistry, the formation and stability of bonds is controlled by geometry, temperature, and pressure. Probing these aspects provides fundamental insight, which leads to an understanding of bonding preferences that could eventually be exploited to manipulate catalytic behavior, and thus custom catalysts.

Scientists at Pacific Northwest National Laboratory have teamed up to understand the nature of the chemical reactivity of titania. Using EMSL's supercomputer, these researchers were able to obtain good agreement with experimental results and new insight into the underlying chemistry. This extensive study was recently published in the American Chemical Society's high-ranking *Journal of Physical Chemistry C*.

The transport of electrons and holes (i.e., the hole left when an electron moves) in titania is well described with a polaron model. Polarons are quasi-particles that consist of an electron or hole and the resulting lattice polarization. In titania, a electron polaron is localized on a titanium site, thereby reducing it to Ti^{3+} , whereas a hole polaron is located on the oxygen site, thereby oxidizing it to O^- . Polarons interact strongly with vibrations and lower their energy by creating a local distortion of the lattice. Polarons can be so small that the

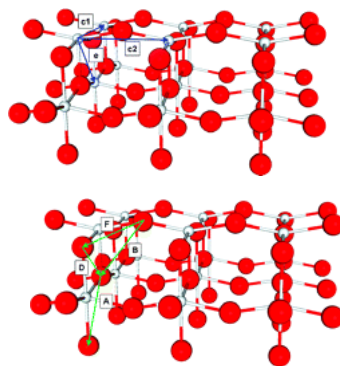


Figure 1. Electron (top) and hole (bottom) polaron transfer directions at the anatase (001) surfaces.



Figure 2. Electron (top) and hole (bottom) polaron transfer directions at the rutile (110) surface.

distortion is smaller than a lattice constant. Polaron transfer in titania is described by a model whereby the reactants (before charge transfer) and products (after charge transfer) potential-energy surfaces are assumed to be parabolic with respect to the reaction coordinate. As the titania is heated, the atoms vibrate more. These thermal fluctuations allow the reactants and products states to interchange freely (i.e. they are energetically degenerate). Such interactions fundamentally change the nature of the material.

The first step in studying polarons was to develop potential parameters for titania based upon energies obtained from density functional theory calculations. These parameters were validated against the extent of lattice distortion of titania crystal lattices upon introduction of electron and hole polarons and the difference in polaron formation energies between rutile and anatase. Good agreement was obtained throughout, and electron polarons have a greater intrinsic affinity for the anatase phase, whereas hole polarons favor the rutile phase. The newly derived potential model was employed in a series of molecular dynamics simulations to investigate the surface effects on the energetics of polaron transfer using the rutile (110) and anatase (001) surfaces. Both the reorganization energy and free energy as a function of depth indicate that the surface effects are limited to the first couple of surface layers at most. However, the topmost surface layer shows large deviations from bulk behavior with increases in reorganization energy varying from approximately 5 to 25 percent and free energies of surface sites up to 3 eV higher than equivalent bulk sites. Polaron transfer directions on the surface are presented in Figures 1 and 2. Although the polaron free energy increases as it approaches the surface, the electrostatic potential of some subsurface sites can be significantly lower than that of equivalent sites in the bulk and thus act as traps for diffusing polarons, as was found for hole polarons at the rutile (110) surface. The presence of these sites may have important implications for the availability of electrons and holes in photocatalytic reactions.

The implications of these discoveries extend beyond just beyond understanding for future energy developments. Titania has also been proposed as a catalyst for the degradation of organic pollutants. The production of nuclear materials has resulted in the release of organic contaminants into the environment at DOE sites. Obtaining an understanding of catalysts that will break down contaminants is a major challenge to the cleanup mission.

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Major Upgrades

Chinook installation. Phase I of the new supercomputer, Chinook, has been installed and user migration has begun.

News Coverage

Rob Farber was interviewed by the Texas Advanced Computing Center for a feature article that should appear on their web site (<http://www.tacc.utexas.edu>) in July.

Awards and Recognition

EMSL User receives M.T. Thomas Award for Postdoctoral Accomplishments. EMSL user **Zhenrong Zhang** (Pacific Northwest National Laboratory) was selected as the 2007 recipient EMSL's M.T. Thomas Award for Outstanding Postdoctoral Achievement. The award recognizes her scientific contributions that promote the mission of EMSL. Her new experimental method and resulting measurements are important steps in material science and may lead, among other things, to designing and controlling catalysts that produce clean-burning hydrogen fuel. She was selected for the award for achieving the first atomically resolved high-temperature scanning tunneling microscopy measurements and resulting insights on the understanding of the adsorbate reactivity and diffusion dynamics on TiO₂. This oxide is an extremely promising material with applications in such diverse and technologically important areas as catalysis, air purification, and wastewater treatment. At EMSL, Zhang designed a new sample heating stage and implemented a breakthrough methodology that resulted in near-perfect TiO₂ surfaces with negligible water contamination. Her methodology was the crucial advance needed to identify the preferred adsorption or adherence sites and dissociation pathways for water and alcohols as well as the diffusion dynamics of surface defects and hydroxyl groups.

EMSL User receives Biemann Medal. EMSL researcher Julia Laskin (Pacific Northwest National Laboratory) received the Biemann Medal, the highest honor granted to a young scientist by the American Society for Mass Spectrometry. Laskin accepted the award at the ASMS annual conference June 3 in Denver. The award recognizes Laskin's contributions to better understanding the activation, fragmentation and deposition of large molecules when they collide with surfaces.

Visitors and Users

During the third quarter of Fiscal Year 2008, a total of 380 users benefited from EMSL capabilities and expertise. This total included 289 onsite users and 101 remote users.

New EMSL Staff

Brock Erwin and Jimmy Wanner of WSU Tri-Cities joined EMSL as summer interns.

Publications

Book Chapters

Wang J, G Liu, and Y Lin. 2008. "Layer-by-Layer Assembly of Enzymes on Carbon Nanotubes." Chapter 6 in *Biomolecular Catalysis Nanoscale Science and Technology*, vol. ACS Symposium Series 986, ed. J. Kim, S. H. Kim, P. Wang, pp. 117-128. American Chemical Society, Washington DC.

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Conferences and Presentations

During the third quarter of Fiscal Year 2008, EMSL staff and users presented on research performed at the user facility or attended conferences at the following meetings or locations:

- 2nd On-Line Particle Mass Spectrometry Workshop, Leeds, United Kingdom, April 9, 2008
- 25th Rare Earth Research Conference, Tuscaloosa, Alabama, June 22-29, 2008
- 213th Electro Chemical Society Conference, Phoenix, Arizona, May 22, 2008
- 235th ACS National Meeting, New Orleans, Louisiana, April 7, 2008

- 2008 Symposium on Radiation Measurements and Applications, Berkeley, California, June 2, 2008
- American Ceramic Society 2008 Glass & Optical Materials Division Meeting, Tucson, Arizona, May 19, 2008
- American Society for Mass Spectrometry Conference, Denver, Colorado, June 1-5, 2008
- DICE Workshop, Mason Ohio, May 6, 2008
- DOE Office of Basic Energy Sciences Principal Investigator Meeting, Richland, Washington, June 11, 2008
- High School Student Research Internship, Richland, Washington, May 22, 2008
- HP-CAST meeting, Singapore, May 21, 2008
- International Symposium on Molecular Spectroscopy, Columbus, Ohio, June 15-20, 2008
- LDRD-RDMD Review, Richland, Washington, June 24, 2008
- LinuxFest Northwest 2008, Bellingham, Washington, April 26, 2008
- NSTI Nanotech 2008, Boston, Massachusetts, June 4, 2008
- Teragrid 2008, Las Vegas, Nevada, June 10, 2008