



EMSL Quarterly Highlights Report
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EMSL—the Environmental Molecular Sciences Laboratory—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

Chemical Speciation of Sulfur in Marine Particles

RJ Hopkins,^(a) Y Desyaterik,^(b) AV Tivanski,^(a) RA Zaveri,^(b) CM Berkowitz,^(b) T Tylicszczak,^(a) MK Gilles,^(a) and A Laskin^(c)

(a) Lawrence Berkeley National Laboratory, Berkeley, California

(b) Pacific Northwest National Laboratory, Richland, Washington

(c) EMSL, Richland, Washington

Detailed chemical speciation of field-collected particles from the marine boundary layer over the California current was performed using a combination of complementary microanalysis techniques. On the basis of composition, morphology, and chemical bonding information, two externally mixed, distinct classes of sulfur-containing particles were identified: chemically modified (aged) sea salt particles and secondary-formed sulfate particles. The results indicate substantial heterogeneous replacement of chloride by methanesulfonate (CH_3SO_3^-) and non-sea-salt sulfate (nss-SO_4^{2-}) in sea-salt particles with characteristic ratios of $\text{nss-S/Na} > 0.10$ and $\text{CH}_3\text{SO}_3^-/\text{nss-SO}_4^{2-} > 0.6$.

A research team of EMSL staff and users presented the first observations of both CH_3SO_3^- and SO_4^{2-} sulfur compounds in marine aerosol, identified on a single-particle basis. Both time-of-flight-secondary ion mass spectrometry (TOF-SIMS) and scanning transmission x-ray microscopy/near-edge x-ray absorption fine structure techniques (STXM/NEXAFS) indicate an external mixture consisting primarily of two particle classes: mixed sea salt/ $\text{CH}_3\text{SO}_3^-/\text{SO}_4^{2-}$ and S-rich particles of mixed $\text{H}_2\text{SO}_4/(\text{NH}_4)_2\text{SO}_4$ composition (Figure 1). Unambiguous, qualitative speciation of sulfur-containing compounds and quantitative assessment of the $\text{CH}_3\text{SO}_3^-/\text{nss-SO}_4^{2-}$ ratios have been facilitated using combined data sets from three techniques: (1) computer-controlled scanning electron microscopy/energy-dispersed X-ray analysis, quantitative assessment of elemental composition of individual particles; (2) TOF-SIMS, qualitative molecular speciation of sulfur-containing

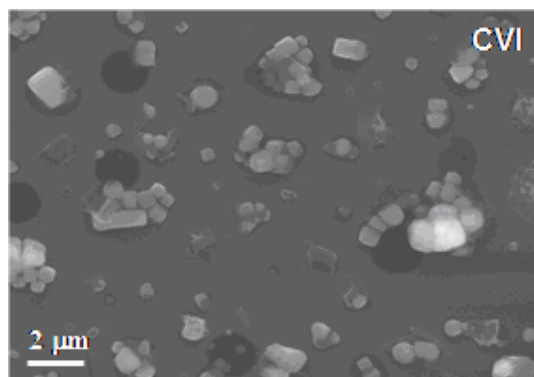


Figure 1. Scanning electron microscopy image of marine particles. Sea-salt particles are larger, irregularly shaped supermicron particles with NaCl cubic crystal cores. Ammonium sulfate particles are spherical submicron particles (Hopkins et al., 2008).

compounds in individual particles; and (3) STXM/NEXAFS, quantitative assessment of different forms of sulfur within individual particles. The data provided by these techniques offer a rich set of qualitative and quantitative information that is of primary importance to atmospheric chemistry processes in the marine boundary layer involving sea-salt and marine sulfate particles.

For the first time, size-dependent nss-S/Na and $\text{CH}_3\text{SO}_3^-/\text{nss-SO}_4^{2-}$ ratios are reported for marine particles. Characteristic ratios of $\text{nss-S/Na} > 0.10$ are reported for sea-salt particles, with higher values observed for smaller particles, indicating more extensive formation of sulfur-containing salts. Characteristic ratios of $\text{CH}_3\text{SO}_3^-/\text{nss-SO}_4^{2-} > 0.60$ are reported for sea-salt particles of all sizes, with higher values for large particles (Figure 2). This indicates that CH_3SO_3^- salts are likely the dominant form of nss-sulfur in large particles, while nss-SO_4^{2-} is more common in smaller particles. In the past, much attention has been given to the hygroscopic and optical properties of sea-salt aerosols and the corresponding mixed sea salt/sulfate particles that can be formed as a result of the $\text{DMS} \rightarrow \text{SO}_2 \rightarrow \text{H}_2\text{SO}_4$ reaction sequence that is assumed to dominate in the mid latitude marine boundary layer. However, our analysis of field-collected sea-salt particles indicate that DMS conversion to MSA can result in $\text{CH}_3\text{SO}_3^-/\text{nss-SO}_4^{2-} > 0.60$ and $\text{nss-S/Na} > 0.1$ ratios, as were observed under specific conditions of the coastal area north of San Francisco. These findings indicate that modeling of the marine boundary layer aerosols and cloud formation processes require extensive data on the hygroscopic and CCN properties of mixed sea salt/ $\text{CH}_3\text{SO}_3^-/\text{SO}_4^{2-}$ and perhaps other organo-sulfur particles. These data are fairly scarce and require future research.

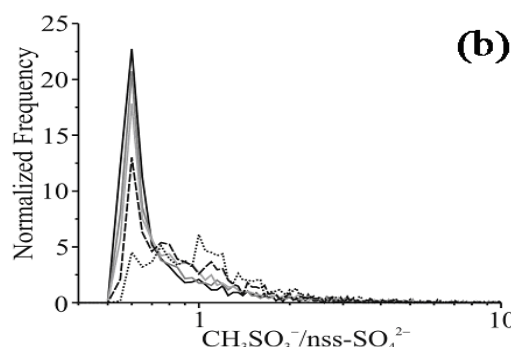


Figure 2. Distribution of CH_3SO_3^- to nss-SO_4^{2-} ratio present in particles with diameter in the range $0.31 - 0.5$, $0.5 - 0.79$, $0.79 - 1.26$, $1.26 - 2$ and $> 2 \mu\text{m}$ (black, dark grey, light grey, dashed and dotted lines, respectively). (Hopkins et al., 2008).

Details of this research were recently published in the *Journal of Geophysical Research – Atmospheres*

Citation

Hopkins RJ, Y Desyaterik, AV Tivanski, RA Zaveri, CM Berkowitz, T Tyliczszak, MK Gilles, and A Laskin. 2008. "Chemical Speciation of Sulfur in Marine Cloud Droplets and Particles: Analysis of Individual Particles from the Marine Boundary Layer over the California Current." *Journal of Geophysical Research D – Atmospheres* 113:D04209, doi:10.1029/2007JD008954.

Application of Methods of High-Resolution Mass Spectrometry to Study Chemistry of Secondary Organic Aerosol

S Nizkorodov,^(a) ML Walser,^(a) AP Bateman,^(a) A Laskin,^(b) J Laskin,^(c) and Y Desyaterik^(c)

(a) University of California, Irvine, California

(b) EMSL, Richland, Washington

(c) Pacific Northwest National Laboratory, Richland, Washington

Methods of high-resolution mass spectrometry have been applied to study chemical composition of secondary organic aerosol (SOA) formed from the ozone-initiated oxidation of limonene. A significantly more complex SOA composition than that predicted by previously reported mechanisms was discovered. A possible reaction mechanism for the formation of the first-generation SOA molecular components has been presented.

High-resolution mass spectrometric characterization of SOA particles formed from the ozone-induced oxidation of limonene revealed that the chemical composition of these particles is significantly more complex than that predicted by the basic Criegee mechanism of alkene ozonolysis. The mass spectra reveal ~1500 condensed products of oxidation, as illustrated in Figure 1. This work convincingly demonstrated that in order to account for the very large number of poly-functional species that exist in SOA in both monomeric and polymeric form, one has to include rich chemistry involving alkylperoxy and alkoxy radicals formed from the decomposition of carbonyl oxide intermediates. The authors described a minimal set of reactions required to produce a distribution of limonene ozonation products that is consistent with mass spectrometric observations. Even with a fairly restrictive set of reaction rules, inclusion of alkylperoxy and alkoxy chemistry in limonene ozonation produces some 1000 products with 140 unique m/z values in the monomeric mass range ($m/z < 300$). The discussed mechanism includes known isomerization and addition reactions of the carbonyl oxide intermediates generated during the ozonation of limonene. In addition, it includes isomerization and decomposition pathways for alkoxy radicals resulting from unimolecular decomposition of carbonyl oxides that have been disregarded by previous studies. The isomerization reactions yield numerous products with a progressively increasing number of alcohol and carbonyl groups, whereas C–C bond scission reactions in alkoxy radicals shorten the carbon chain. Together these reactions yield a large number of isomeric products with broadly distributed masses. A qualitative agreement is found between the number and degree of oxidation of the predicted and measured reaction products in the monomer product range.

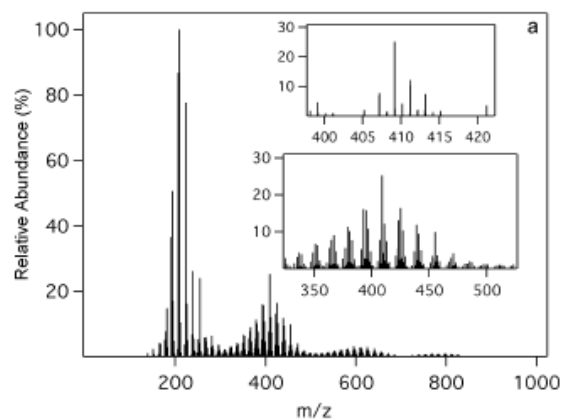


Figure 1. Representative positive ESI mass spectra of SOA particles extracted in acetonitrile. The data include peaks with >0.5% abundance relative to the largest peak in the spectrum. (Walser et al., 2008).

The large number of isomeric products produced in the oxidation of just one terpene shows how challenging it will be to obtain detailed characterization of molecular composition of ambient SOA particles that typically result from oxidation of multiple precursors. The ultimate goal of research on chemical mechanisms of SOA formation is to find out which reactions out of the infinite number of possibilities actually take place, and

which are likely to be insignificant. It is expected that for such complex systems, the answer to this question will come from coupling mass spectrometry and information theory, and this work can be viewed as the first step in that direction.

Details of this research were recently published in *Physical Chemistry Chemical Physics*.

Citation

Walser ML, Y Desyaterik, J Laskin, A Laskin, and SA Nizkorodov. 2008. "High-Resolution Mass Spectrometric Analysis of Secondary Organic Aerosol Produced by Ozonation of Limonene" *Physical Chemistry Chemical Physics* 10(7):1009-1022.

Laboratory Studies on the Effect of Primary Organic Aerosols on Secondary Organic Aerosol Formation

M. Elizabeth Alexander,^(a) Chen Song,^(b) Rahul A. Zaveri,^(b) Joel A. Thornton,^(c) Alla Zelenyuk,^(b) Xiao-Ying Yu,^(b) Sasha Madronich,^(d) and David Maughan^(b)

(a) EMSL, Richland, Washington

(b) Pacific Northwest National Laboratory, Richland, Washington

(c) University of Washington, Seattle, Washington

(d) National Center for Atmospheric Research, Boulder, Colorado

The effect of existing primary organic aerosols (POA), typical of automobile and truck emissions, on the formation of secondary organic aerosol (SOA) is investigated in a controlled laboratory setting. The results of these studies showed no enhancement of SOA yields by POA, in sharp contrast to assumptions inherent in current atmospheric models for SOA production, pointing to a need for more sophisticated understanding of the chemical and physical processes underlying SOA formation in the atmosphere.

A suite of EMSL instrumentation was used in fundamental laboratory studies to evaluate the effect of primary organic aerosol (POA) on secondary organic aerosol (SOA) yields in a laboratory-based smog chamber. The EMSL proton transfer reaction mass spectrometer was used to measure the gas-phase concentrations of α -pinene and reaction products resulting from ozonolysis. Particle number concentrations were monitored with a standard scanning mobility particle size, while real-time size, composition and mass concentration were monitored with the EMSL time-of-flight aerosol mass spectrometer. Density of α -pinene SOA particles was measured in independent experiments using the EMSL single-particle laser-ablation time-of-flight mass spectrometer. Dioctylphthalate (DOP) and lubricating oil were used as surrogate POA seed aerosols, and oxidation of α -pinene by ozonolysis was used as a controlled SOA formation mechanism. All measurements were made in an indoor 8 m³ Teflon smog chamber at PNNL.

Representative aerosol mass spectra from lubricating oil, pure α -pinene SOA particles, and α -pinene SOA formed with lubricating oil particles present are shown in Figure 1. These spectra can be qualitatively interpreted using the ratio of molecular fragments at m/Z 57 (C₄H₉⁺) to 44 (CO₂⁺) to indicate the ratio of hydrocarbon-like aerosol (HOA) to oxygenated organic aerosols (OOA). As expected, the ratio is much higher, 8.9 for lubricating oil than for the more highly oxidized α -pinene SOA. The third mass spectrum is for the mixture of lubricating oil and α -pinene and is a nominal value. Figure 2 shows the time evolution

of the ratio HOA /OOA derived from a statistical analysis of the time-resolved aerosol mass spectra as SOA is formed from ozonolysis.

Figure 3 (symbols) shows a plot of observed SOA mass for the entire study with no seed, lube oil seed and with DOP seed. The SOA yield (Y) is defined as $Y = \Delta[\alpha\text{-pinene}]$, where M_{SOA} ($\mu\text{g m}^{-3}$) is the mass concentration of SOA formed and $\Delta[\alpha\text{-pinene}]$ ($\mu\text{g m}^{-3}$) is the amount of α -pinene reacted with ozone. Also shown are the results of the two-product, semi-empirical Odum model equation, currently the basis for atmospheric SOA models (e.g., Chung and Seinfeld 2002) in the absence of any seed aerosols.

Note that all the M_{SOA} observations for these studies fall on the same baseline curve that was obtained for the unseeded experiments. These results indicate that in the presence of DOP and lubricating oil seed, aerosols do not enhance the formation of SOA mass by providing additional absorbing mass. It therefore appears that the condensed SOA species form a separate organic phase, which then behaves in the same manner as the homogeneously nucleated SOA with regard to the gas-particle partitioning coefficients. Current atmospheric SOA models, based on these results, may erroneously predict high SOA yields. If these results apply to other SOA precursors, the current under-prediction of SOA by current atmospheric models compared to field measurements is more severe than previously believed. This conclusion underscores the need for molecular-level laboratory studies to fully understand the actual chemical and physical processes for SOA formation in the ambient atmosphere at urban, regional, and global scales.

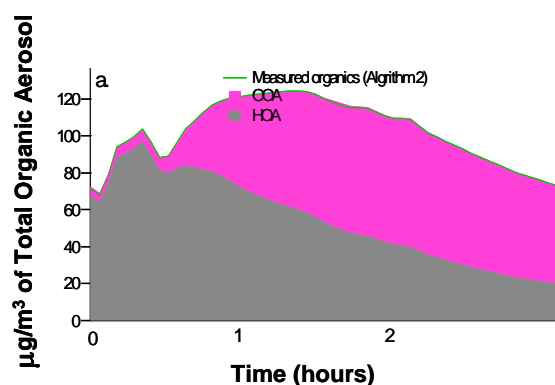


Figure 2. Time evolution of POA and SOA fractions during oxidation of α -pinene in the presence of lubricating oil seed.

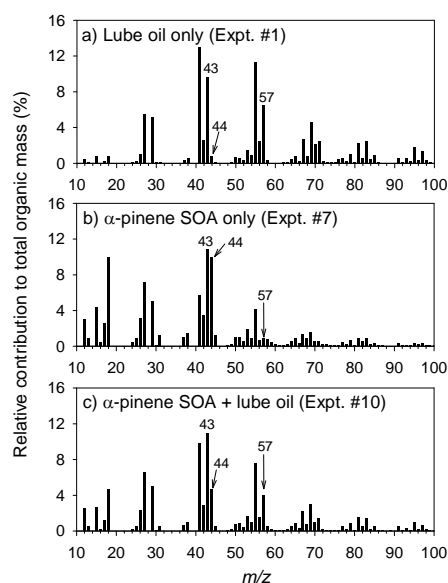


Figure 1. Representative normalized AMS spectra for (a) lubricating oil, (b) α -pinene and (c) α -pinene with lubricating oil (Song et al 2007).

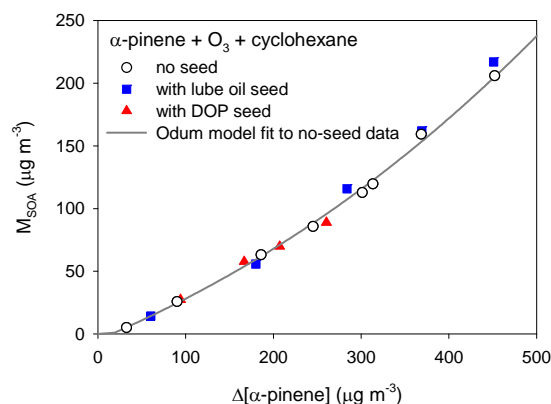


Figure 3. Comparison of SOA mass produced in the absence and presence of DOP and lubricating oil seed aerosols as a function of amount of α -pinene reacted with fit from Odum model. (Song et al 2007)

Details of this research were recently published in *Geophysical Research Letters*.

Song C, RA Zaveri, ML Alexander, JA Thornton, S Madronich, JV Ortega, A Zelenyuk, XY Yu, A Laskin, and DA Maughan. 2007. "Effect of Hydrophobic Primary Organic Aerosols on Secondary Organic Aerosol Formation from Ozonolysis of α -pinene." *Geophysical Research Letters* 34: L20803, doi:10.1029/2007GL030720.

Chung SH, and JH Seinfeld. 2002. "Global Distribution and Climate Forcing of Carbonaceous Aerosols." *Journal of Geophysical Research* 107(D19):4407, doi:10.1029/2001JD001397.

Biological Interactions and Dynamics

NMR Bioreactor Development for Live In-Situ Microbial Functional Analysis

PD Majors^(a), JS McLean^(b), and JCM Scholten^(c)

(a) Pacific Northwest National Laboratory, Richland, Washington

(b) The J. Craig Venter Institute, La Jolla, California

(c) Merck Co., Inc., West Point, Pennsylvania

An NMR bioreactor developed by EMSL users yields accurate metabolite profiles, metabolic pathways, and reaction rates without altering or depleting the sample. This research is one example of EMSL's move from static to dynamic studies in native environments.

Feeding microbes waste and having them convert it into valuable chemicals may sound far fetched, but scientists are closer, thanks to a new technology developed at EMSL. A first-of-its-kind MRI bioreactor (Figure 1) provides accurate metabolic information for live cells maintained in a controlled growth environment. Similar to clinical MRI, this *improved* technology uses noninvasive (nuclear) magnetic resonance imaging and spectroscopy (MRI/MRS) methods to monitor microbial metabolite concentrations *in the reactor* without removal or processing. This new technology provides a major advantage because metabolite levels can change significantly due to handling. Further, this technology allows for frequent, repeating measurements without diminishing the sample. Finally, it is compatible with high-throughput genomic and proteomic analyses.

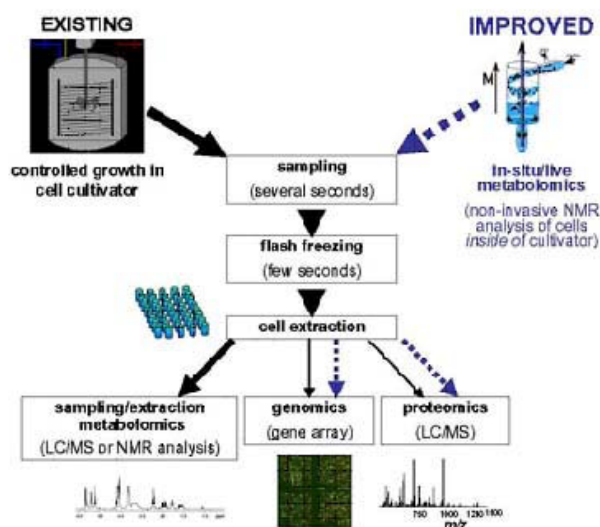


Figure 1. The conventional technology (left) compared to the improved technology (right).

The MRI/MRS bioreactor was used to study metabolites produced by *Eubacterium aggregans*, an anaerobic bacterium of interest for bio-fuel production. The study showed that in addition to known metabolic byproducts -- *E. aggregans* produces significant concentrations of lactate, a metabolite not previously reported. This suggests that the activities of its metabolic networks are different from what were predicted based on older experimental techniques. This research was featured on the cover of *Journal of Magnetic Resonance*.

Citation

Majors PD, JS McLean, and JC Scholten. 2008. "NMR Bioreactor Development for Live In-Situ Microbial Functional Analysis." *Journal of Magnetic Resonance* 192(1):159-166.

The Structure of the GAF A Domain from Phosphodiesterase 6C Reveals Determinants of cGMP-Binding, a Conserved Binding Surface, and a Large cGMP-Dependent Conformational Change

SE Martinez^(a), CC Heikaus^(a), RE Klevit^(a), and JA Beavo^(a)

(a) University of Washington, Seattle, Washington

Determining the first structure of the photoreceptor phosphodiesterase bound to its ligand, cyclic guanosine monophosphate, is an important step for understanding ocular function. Studies such as this one support EMSL's goal to measure dynamic interactions in native environments and to predict biological functions from molecular and chemical data.

The eyes house the elegant machinery that responds to photons and triggers the neural impulses that allow us to visualize our environment. Researchers from the University of Washington have used EMSL's nuclear magnetic resonance spectrometers and sophisticated probe technologies to gain new knowledge about the complex visual system at the molecular level. The team is the first to determine a high-resolution structure of the regulatory domain of the photoreceptor phosphodiesterase (PDE6) bound to its ligand, cyclic guanosine monophosphate (cGMP) (Figure 1). Studies such as this one are the first steps toward a fundamental understanding of how the visual system works and how to fix it when it goes awry.

The interaction between PDE6 and cGMP affects how *quickly* the eye can see. When it is activated by light, the regulatory region of PDE6, referred to as GAF A, activates PDE6. PDE6 in turn degrades cGMP, ultimately allowing the brain to receive information from the retina. Previous attempts to learn more about the ligand-free PDE6 GAF A domain via crystallization and diffraction studies were unsuccessful because crystals of the ligand-free protein are not easily prepared. So,

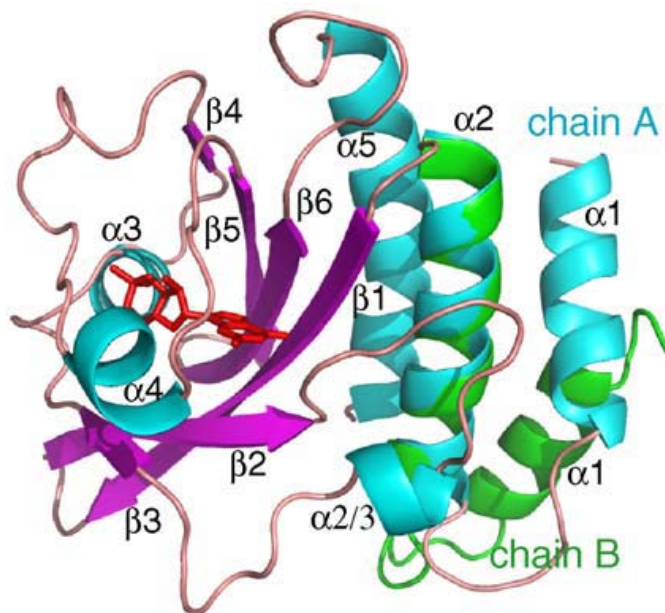


Figure 1. Structure of PDE6 GAF A bound to cGMP (red).

the team turned to EMSL's NMR spectrometer and probe capabilities to investigate the conformational change of recombinant PDE6 while binding cGMP in real time and confirmed, at the atomic level, that GAF A is indeed the PDE6 binding site of cGMP.

This research was featured on the cover of *The Journal of Biological Chemistry*.

Citation

Martinez SE, CC Heikaus, RE Klevit, and JA Beavo. 2008. "The Structure of the GAF A Domain from Phosphodiesterase 6C Reveals Determinants of cGMP-Binding, a Conserved Binding Surface, and a Large cGMP-Dependent Conformational Change" *The Journal of Biological Chemistry* doi 10.1074/jbc.M802891200.

Backbone ^1H , ^{13}C , and ^{15}N NMR Assignments for the *Cyanothece* 51142 Protein *cce_0567*: A Protein Associated with Nitrogen Fixation in the DUF683 Family

GW Buchko^(a) and HJ Sofia^(a)

(a) Pacific Northwest National Laboratory, Richland, Washington

Understanding the structure of cce_0567 and other cyanobacteria proteins paves the way for further scientific inquiry, including biochemical experiments, into ubiquitous blue-green algae. This research is an example of EMSL's efforts to uncover biological functions from molecular and chemical data.

As part of EMSL's Membrane Biology Grand Challenge, users have determined the crystal structure for the 78-residue protein *cce_0567* from the cyanobacteria *Cyanothece* sp. PCC 51142. Studies suggest that the protein may play a role in nitrogen fixation and/or the circadian control of nitrogen fixation. Nitrogen fixation is the rate-limiting step in the growth of cyanobacteria. Understanding the proteins involved in nitrogen fixation could help unlock the mysteries of how to efficiently turn this ubiquitous algae into a carbon-neutral fuel.

Using EMSL's state-of-the-art resources, the nuclear magnetic resonance chemical shift assignments for *cce_0567* were made using EMSL's 500-, 600-, 750-, and 800-MHz NMR spectrometers. The ^1H - ^{15}N HSQC spectrum is a "fingerprint" for the protein's conformation. The assignment of the ^1H - ^{15}N HSQC spectrum is an important step in probing the biological function of *cce_0567* (Figure 1). Perturbations to these chemical shifts occur when other molecules are added to the solution. The perturbations are indicative of substrate binding. Following such chemical shifts allows researchers to identify protein-substrate interactions and then map them on to specific locations on the protein's surface using the structure determined by crystallographic methods. This research was published in *Biomolecular NMR Assignments*.

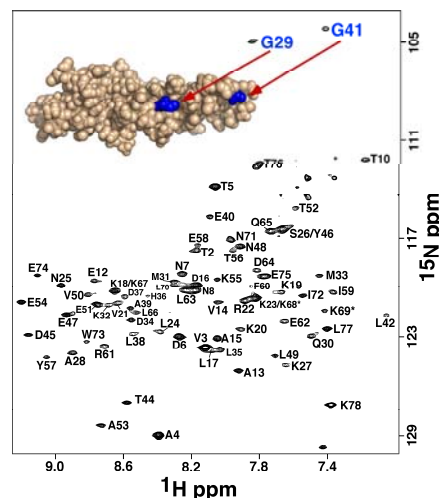


Figure 1. The assigned ^1H - ^{15}N HSQC spectrum for *cce_0567* with the crystal structure of the protein (3CSX) is shown near the top. Understanding the function of this protein may help scientists use blue-green algae for producing energy and sequestering carbon.

Citation

Buchko GW, and HJ Sofia. 2008. "Backbone ¹H, ¹³C, and ¹⁵N NMR Assignments for the *Cyanotheca 51142* Protein cce_0567: A Protein Associated with Nitrogen Fixation in the DUF683 Family." *Biomolecular NMR Assignments* 2(1):25-28.

Trapped-Ion Cell with Improved DC Potential Harmonicity for FT-ICR MS

AV Tolmachev^(a), EW Robinson^(a), S Wu^(b), H Kang^(b), NM Lourette^(a), L Pasa-Tolic^(c), and RD Smith^(a)

^(a) Pacific Northwest National Laboratory, Richland, Washington

^(b) Ajou University, Suwan, Korea

^(c) EMSL, Richland, Washington

Using a more homogenous electric field in the FTICR, a mass spectrometric cell developed at EMSL is providing a two-fold increase in ion characterization. This work supports studies at EMSL to predict biological functions from molecular and chemical data.

Whether studying proteins to identify methods for less invasive medical tests or discover hydrocarbons for new energy sources, scientists need instruments that provide reliable, accurate measurements. A new trapped-ion cell, designed and developed at EMSL, provides a two-fold improvement in mass accuracy. This increased accuracy allows scientists to more confidently analyze highly complex mixtures and distinguish between nearly identical molecules in samples.

The cell (Figure 1), designed by scientists from Pacific Northwest National Laboratory, Ajou University, and EMSL, is being used on several proteomics research projects in combination with EMSL's 12-Tesla Fourier transform ion cyclotron resonance mass spectrometer. The scientists began by studying the theories underlying FTICR and the accuracy obtained. Critical to the success of this mass spectrometry technique is the cell where the ions are trapped and excited. The new design generates an electrostatic trapping potential, responsible for holding the ions, that closely approaches the theoretical ideal. The new cell allows for

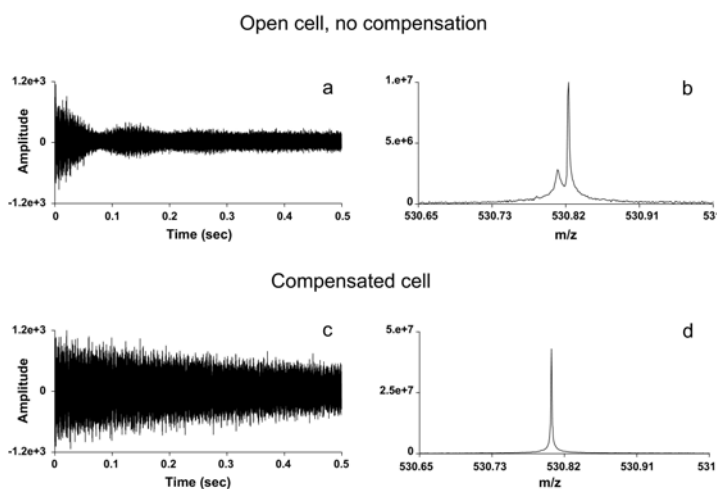


Figure 1. Peptide ions, coherently excited, induce a current on two detection plates using a conventional open cell (top left) and the new cell (bottom left). The more the ions are excited, the closer they get to the detection plates, which should increase the measured signal. However, in the open cell (top right), non-ideal electric fields distort the ion motion, resulting in peak splitting, reduced mass measurement accuracy, and reduced sensitivity. The more theoretically ideal electric fields in the new cell enable ions to be excited closer to the detection plates with significantly less distortion of the ion motion improving sensitivity (peak amplitude), dynamic range, and mass measurement accuracy. These improvements will result in more peptides (and therefore more proteins, especially less abundant proteins) being identified with greater confidence.

higher signals and thus increased sensitivity and dynamic range. Experimental characterization of the new cell confirmed that a more homogeneous electrostatic trapping field improves the FTICR's performance. This research was featured in *Journal of the American Society of Mass Spectrometry*.

Citation

Tolmachev AV, EW Robinson, S Wu, H Kang, NM Lourette, L Pasa-Tolić, and RD Smith. 2008. "Trapped-Ion Cell with Improved DC Potential Harmonicity for FT-ICR MS." *Journal of the American Society of Mass Spectrometry* 19(4):586-97.

Functional and Structural Characterization of DR_0079 from *Deinococcus radiodurans*, a Novel Nudix Hydrolase with a Preference for Cytosine (Deoxy)Ribonucleoside 5'-Di- and Triphosphates

GW Buchko^(a), O Litvinova^(b), H Robinson^(c), AF Yakunin^(b), and MA Kennedy^(d)

(a) Pacific Northwest National Laboratory, Richland, Washington

(b) University of Toronto, Toronto, Ontario, Canada

(c) Brookhaven National Laboratory, Upton, New York

(d) Miami University, Oxford, Ohio

*A new function documented for a Nudix hydrolase of *D. radiodurans*, DR_0079, expands the range of possible Nudix substrates and provides an understanding of the molecular basis for *D. radiodurans* radiation-resistant properties, which may lead to novel bioremediation methods and to strategies that protect humans from the deleterious effects of ionizing radiation. Novel findings from real-time, molecular-level structure-function studies further EMSL's goals to predict biological functions from molecular and chemical data and to advance from static to dynamic studies in native environments.*

Deinococcus radiodurans can survive thousands of times more radiation exposure than a human. The biological mechanism for its radiation resistance may be related to an uncommonly large suite of housekeeping proteins called Nudix hydrolases. A research team from Brookhaven National Laboratory, the University of Toronto, Miami University, and Pacific Northwest National Laboratory have used EMSL's state-of-the-art nuclear magnetic resonance spectroscopy capabilities to help determine the crystal structure for one of these *D. radiodurans* Nudix hydrolases, DR_0079, and uncovered its preference for a novel substrate (Figure 1).

Nudix hydrolases are ubiquitous, existing in the genomes of organisms as diverse as viruses and humans. They are identified by a highly conserved, 23-residue consensus sequence, called the Nudix box, which forms part of the substrate-binding and catalytic site. The rest of a Nudix hydrolase's sequence determines the overall protein structure, which in turn influences substrate specificity. Substrates for Nudix hydrolases are typically nucleotide-based (related to the

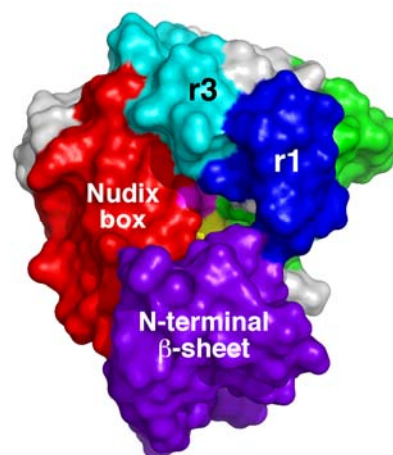


Figure 1. DR_0079 (205F) surface structure highlighting the Nudix box (red) and regions of the protein associated with substrate binding.

building blocks of DNA and RNA). The classic Nudix protein, MutT, protects cells by converting dangerous promutagenic nucleoside triphosphates into safe nucleoside monophosphates – the former can be incorporated into DNA and lead to cancer, and the latter cannot. DR_0079 is unusual because it converts nucleoside *diphosphates* instead of nucleoside triphosphates into nucleoside monophosphates.

The team used X-ray diffraction data collected at the National Synchrotron Light Source to study the structure of DR_0079. To relate structure to function, the preferred substrate of the enzyme was verified and the molecular mechanism probed using ³¹P NMR spectroscopy at EMSL. This technique made it possible to study the protein's activity in real time and with molecular detail. This research was reported in *Biochemistry*.

Citation

Buchko GW, O Litvinova, H Robinson, AF Yakunin, and MA Kennedy. 2008. "Functional and Structural Characterization of DR_0079 from *Deinococcus radiodurans*, a Novel Nudix Hydrolase with a Preference for Cytosine (Deoxy)Ribonucleoside 5'-Di- and Triphosphates." *Biochemistry* 47:6571-82.

Researchers integrate computing with experiments to gain insight in the structure and function of enzymes and peptides

EMSL's experimental capabilities, combined with its computational modeling capabilities, provides fundamental insight into the structure and function of enzymes and proteins. This knowledge is essential for understanding the inner workings of biological systems.

One of EMSL's key characteristics is the integration of state-of-the-art experimental and computational capabilities. With all these capabilities under one roof, EMSL enables researchers to get access to a broad range of capabilities to solve some of the most important national challenges in energy, environmental sciences, and human health in a multidisciplinary fashion. Computational chemistry combined with large supercomputers has reached a level of accuracy such that simulations can help researchers interpret and understand complex experimental observations, or even guide experiments. Here two examples are highlighted where researchers have used experimental NMR or FT-CIR capabilities in conjunction with EMSL's NWChem software and supercomputer to gain knowledge about the inner working of biological systems.

Researchers from the University of Michigan and Pacific Northwest National Laboratory recently published an article in the top-ranking *Journal of the American Chemical Society*, describing how a combination of NMR experiments and insights from computational chemistry simulations lead to a detailed understanding of the structure and behavior of the Aquifex aeolicus LpxC enzyme in different environmental conditions. The scientists used EMSL's 500 and 800 MHz NMR and the NWChem software on EMSL's supercomputer to accomplish their research. Experiments have shown that the LpxC enzyme, which has a catalytic zinc ion in its center, reacts differently depending on pH. The main goal of this research was to identify at which pH the zinc-bound water of the enzyme, and also at which pH other parts of the enzyme get ionized. By calculating the NMR properties for

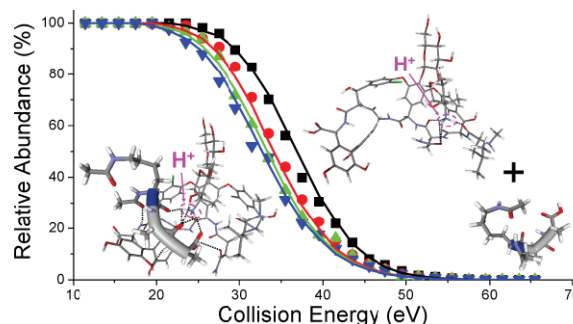


Figure 1. Fragmentation of the charged vancomycin-peptide complex (left) forms a protonated vancomycin and a neutral peptide molecule.

various ionized enzyme structures, and comparing them with experimental data they were able to conclude that the water bound to the zinc ion in fact does not get ionized at all. Instead they found that two different side chains get deprotonated depending on the pH level.

Another article in the *Journal of the American Chemical Society*, researchers from Pacific Northwest National Laboratory demonstrated how the integration of theory and experiment can lead to a molecular-scale understanding of noncovalent interactions in biomolecular systems. In their research the scientists did surface-induced dissociation (SID) experiments with EMSL's 6 Tesla Fourier transform ion cyclotron resonance mass spectrometer (FT-ICR MS) configured for studying ion-surface collisions, and theoretical calculations using EMSL's NWChem software and supercomputer. To probe the interaction of the vancomycin antibiotic with an analogue of a cell wall peptide (N_aN_c-diacetyl-L-Lys-D-Ala-D-Ala), the researchers collided a protonated vancomycin-peptide complex with a surface to break it apart. This experiment allows them to obtain the binding energy between vancomycin and the peptide. Computational chemistry simulations were used to interpret the structure and composition of the complex. Comparison of binding energies obtained from different complexes modeled with theory and experiment provided the unique insight that the protonated complex really consists of a neutral peptide while the disaccharide group in vancomycin is protonated.

Citations

Lipton AS, Heck RW, Hernick M, Fierke CA, and Ellis PD. 2008. "Residue Ionization in LpxC Directly Observed by ⁶⁷Zn NMR Spectroscopy" *Journal of the American Chemical Society* 130: 12671-12679

Yang Z, Vorpapel ER, and Laskin J. 2008. "Experimental and Theoretical Studies of the Structures and Interactions of Vancomycin Antibiotics with Cell Wall Analogues" *Journal of the American Chemical Society* 130: 13013-13022

Geochemistry/Biogeochemistry and Subsurface Science

In Vitro Evolution of a Peptide with a Hematite Binding Motif That May Constitute a Natural Metal–Oxide Binding Archetype

BH Lower^(a), RD Lins^(a), ZW Oestreich^(b), TP Straatsma^(a), MF Hochella, Jr. ^(c), L Shi^(a), and SK Lower^(b)

(a) Pacific Northwest National Laboratory, Richland, Washington

(b) The Ohio State University, Columbus, Ohio

(c) Virginia Tech, Blacksburg, Virginia

This research answers a fundamental question in polypeptide binding and could aid researchers in everything from better understanding geochemical processes to designing and controlling material synthesis for biofuel cells. This work is part of EMSL's continued effort to link theory and simulations to experiments in real time.

A diverse team of geologists, biologists, and computer scientists from the Pacific Northwest National Laboratory, The Ohio State University, and Virginia Tech is looking into how microorganisms bind to iron oxide. These interactions, common in the subsurface, are of importance to understanding the transport of

environmental contaminants and subsequent remediation. Using computational and experimental resources at EMSL, the team found the protein fragment or polypeptide, just 9 amino acids long, that glues the larger protein to iron oxide.

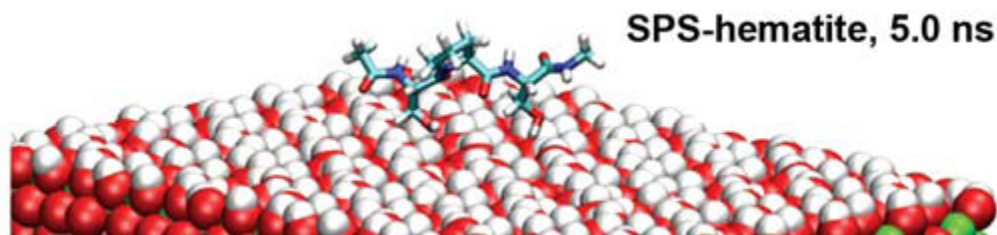


Figure 1. Snapshot of the SPS-hematite simulation at 5.0 ns. The peptide adopts a conformation that allows its two serine residues to form hydrogen bonds with hematite and template the iron oxide surface.

To find this binding polypeptide, the team began with phage technology, using a virus to create more than 3 billion different polypeptides. They screened these molecules and found the polypeptide that would bind to hematite. Next, they performed molecular simulations using an AMBER96 force field with EMSL's NWChem. The simulations showed that the polypeptide takes on a shape that matches the mineral surface, allowing it to grip the surface (Figure 1). Finally, the team searched the genomes of numerous bacteria to see if the polypeptide existed in microbes known for their interactions with metal oxides and found the sequence in *Thalassiosira pseudomonas* and *Shewanella oneidensis*. This research was featured in *Environmental Science and Technology*.

Citation

Lower BH, RD Lins, ZW Oestreich, TP Straatsma, MF Hochella, Jr., L Shi, and SK Lower. 2008. "In Vitro Evolution of a Peptide with a Hematite Binding Motif That May Constitute a Natural Metal-Oxide Binding Archetype." *Environmental Science and Technology* 42(10):3821-3827.

Science of Interfacial Phenomena

A Multinuclear MAS NMR Investigation of the Environmentally Relevant Material Magnesium Aluminum Layered Double Hydroxides

JL Palumbo,^(a) PJ Sideris,^(a) and CP Grey^(a)

(a) State University of New York at Stony Brook, Stony Brook, New York

Magnesium aluminum layered double hydroxides serve as an anion exchange material that can remove toxic anions such as selenates, arsenates and halides from wastewater. The detailed structure of these materials has been unknown, and this work uses nuclear magnetic resonance to determine their structure, which is important to understanding how to develop new materials that are more selective or effective in the role of treating wastewater. The results of this research were reported in Science.

The anion-exchange ability of layered double hydroxides (LDHs) has been exploited to create materials for use in catalysis, drug delivery, and environmental remediation. The specific cation arrangements in the

hydroxide layers of hydrotalcite-like LDHs, of general formula $\text{Mg}^{2+}_{1-x}\text{Al}^{3+}_x\text{OH}_2(\text{Anion}^{n-}_{x/n})\cdot y\text{H}_2\text{O}$, have, however, remained elusive, and their elucidation could enhance the functional optimization of these materials. The presence of a trivalent metal in the metal hydroxide $[\text{M}_{1-x}\text{M}'_x(\text{OH})_2]$ sheet induces an overall positive charge, which is compensated by the incorporation of the anion, along with structural water, in the interlayer spaces (Figure 1). One naturally occurring example of this class of materials is the mineral hydrotalcite, $\text{Mg}_6\text{Al}_2(\text{OH})_{16}\text{CO}_3\cdot 4\text{H}_2\text{O}$, which contains carbonate ions in between the layers. The use of several nuclear magnetic resonance (NMR) techniques, including high-speed magic angle spinning (MAS), Multiple Quantum MAS (MQMAS), and high-field NMR spectra on a 900-MHz spectrometer have combined to give a clear picture of the atomic organization of hydrotalcite which has not been possible using other techniques. We looked at several compositions of hydrotalcite with varying amounts of aluminum, up to 33% aluminum on a molar ratio, so we could compare how the spectra changed with composition. Particular attention was paid to the naturally occurring form with a 2:1 ratio of magnesium to aluminum. If the metal sites were randomly distributed, there would be a distribution of the hydroxide sites with 1, 2, 3 or 4 nearest aluminum neighbors. The NMR data indicate that the hydroxide sites are next to either 0 or 1 aluminum neighbors, indicating that the aluminum sites are not randomly distributed, but are part of an ordered structure where no more than one aluminum site is near a hydroxide group.

21.1-Tesla (900-MHz) NMR data from magnesium samples of brucite ($\text{Mg}(\text{OMg})_6$), 19% aluminum, 25% aluminum, and 33% Al LDH's show that both the brucite and the 33% aluminum LDH have strong axial symmetry, but the quadrupolar properties of the magnesium are different between the two samples. This indicates that the magnesium spectrum is sensitive to the addition of aluminum to the structure, even though the overall structure is not changed by the substitution of aluminum for magnesium. The magnesium NMR data from the intermediate concentrations of aluminum show the presence of both the brucite signal and the 33% aluminum LDH signal, demonstrating a nice transition between forms as more aluminum is added to the material.

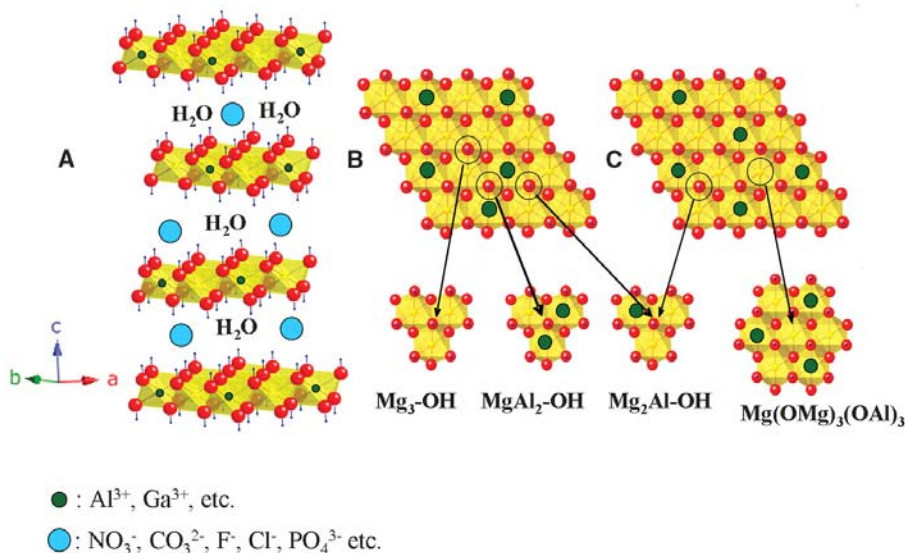


Figure 1. (A) A polyhedral representation of the LDH structure showing the metal hydroxide octahedra stacked along the crystallographic c axis. Water and anions are present in the interlayer region. Each hydroxyl group (dark blue) is oriented toward the interlayer region and may be hydrogen-bonded to the interlayer anions and water. The metal hydroxide sheets of an LDH with a Mg:Al ratio of 2:1 are shown with (B) random and (C) ordered cation distributions. Three major classes of hydroxyl groups are present in (B) ($\text{Mg}_3\text{-OH}$, $\text{Mg}_2\text{Al-OH}$, and $\text{MgAl}_2\text{-OH}$), whereas only one hydroxyl environment ($\text{Mg}_2\text{Al-OH}$) and one Mg local environment [$\text{Mg}(\text{OMg})_3(\text{OAl})_3$] are present in (C).

Figure 1 demonstrates the structure of the 33% aluminum LDH with the bound anions between the sheets of the LDH in A. B shows a random distribution of hydroxide groups, which is not what was found, and C shows the ordered arrangement which was discovered.

Citation

Sideris PJ, UG Nielsen, Z Gan, and CP Grey. 2008. "Mg/Al Ordering in Layered Double Hydroxides Revealed by Multinuclear NMR Spectroscopy." *Science* 321(5885):113-117.

Nuclear-spin Relaxation of ^{207}Pb in Ferroelectric Powders

LS Bouchard^(a), AO Sushkov^(b), D Dudker^(a,b), JJ Ford^(c), and AS Lipton^(d)

(a) Lawrence Berkeley National Laboratory, Berkeley, California

(b) University of California at Berkeley, Berkeley, California

(c) EMSL, Richland, Washington

(d) Pacific Northwest National Laboratory, Richland, Washington

Certain fundamental properties of matter are still not fully understood at the atomic and subatomic level. One such property is the Schiff moment, which can be present in high atomic weight nuclei and violates the parity (P) and time reversal (T) symmetries of standard quantum mechanics. Materials with high ferroelectric moments, such as lead titanates, present the opportunity to measure a Schiff moment on a macroscopic scale. However, there is a lot of preliminary work needed before the Schiff moment can be observed and measured, including the work presented here.

Motivated by a recent proposal by Sushkov and co-workers to search for a P,T-violating Schiff moment of the ^{207}Pb nucleus in a ferroelectric solid, we have carried out a high-field nuclear magnetic resonance study of the longitudinal (T_1) and transverse (T_2) spin relaxation of the lead nuclei from room temperature down to 10 K for powder samples of lead titanate (PT), lead zirconium titanate (PZT), and a PT monocrystal.

Ferroelectric solids have unique properties, including the presence of a macroscopic electric field, which makes them useful in many electronic devices, including sensors. Their properties also make them suitable to observe and measure the presence of a P,T violating Schiff moment. The temperature range to be studied was from room temperature down to 10K. As the samples cooled, the T_1 should increase and the rate of increase would be a reflection of the relaxation processes involved. With the need to vary the temperature over such a wide range, there is very little equipment capable of making this measurement. However, a custom probe designed and built at EMSL has the required range for this set of experiments, and we were able to make use of this unique resource for these experiments.

T_2 data collected over the entire temperature range indicated a constant T_2 of about 1 ms for all samples. This is consistent with a dipole-dipole relaxation mechanism for T_2 relaxation. As seen in Figure 1, the T_1 data is considerably more interesting. At temperatures above 50 Kelvin, all of the samples had a linear relationship between temperature and relaxation rate ($1/T_1 \propto T^2$). This is characteristic of a two-phonon Raman process, a relaxation mechanism investigated and explained in terms of modulation in the spin-rotation interaction. There is a temperature (the Debye temperature) below which this process would become dependent T^7 . The T_1 data below 50K does not follow this behavior, but instead follows a more complicated behavior. This behavior is consistent with paramagnetic impurities being present in the samples and, at low temperatures,

this becomes the dominant source of T_1 relaxation. Over the course of the temperature range, the T_1 increases from 10 seconds at room temperature to one hour at 10K. These research results were reported in *Physical Review A*.

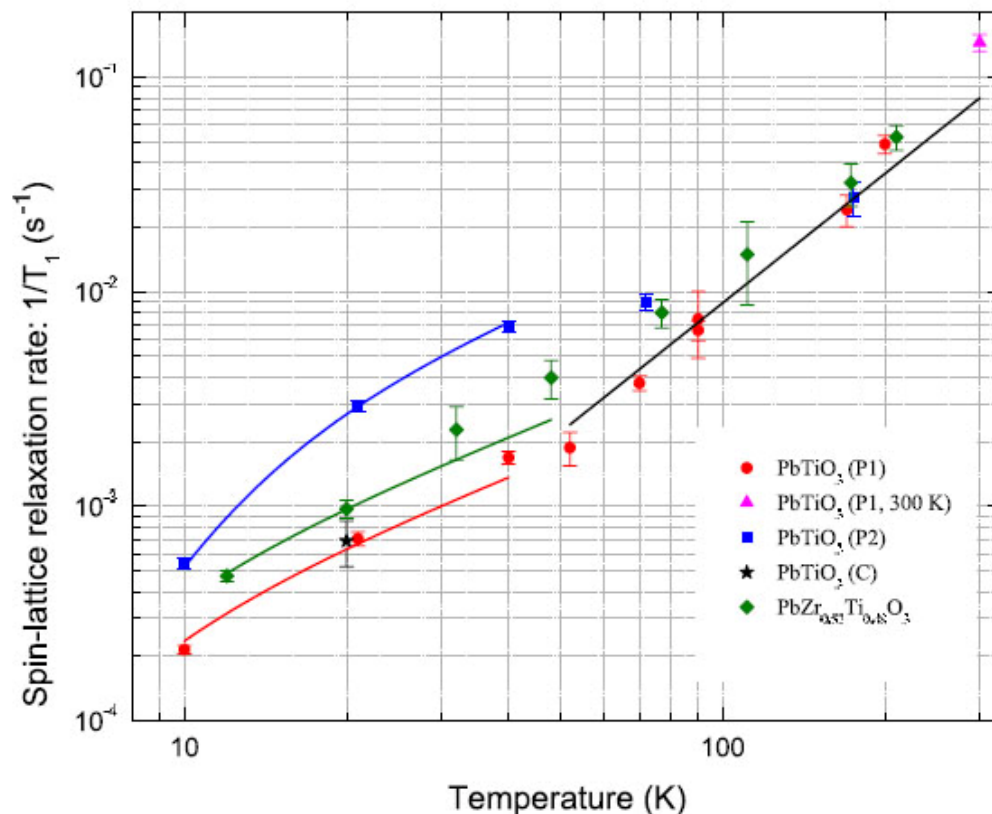


Figure 1. Graph of Relaxation rate ($1/T_1$) versus temperature.

The presence of paramagnetic impurities may actually be useful in the effort to observe Schiff moments in using ^{207}Pb nuclear magnetic resonance. To observe the Schiff moment, the temperature needs to be dropped to less than 1K. This would be done by cooling the sample to 1K and then demagnetize the sample to cool it further. A one-hour T_1 is convenient because that is not too long to achieve full polarization of the sample, but long enough to make the necessary measurements to observe the Schiff moment. Two main questions remain to be answered in future investigations: what is the spin-lattice relaxation time in low magnetic fields and low spin temperatures, and does the presence of paramagnetic impurities introduce serious systematics into the Schiff-moment-induced magnetization search? We are currently developing experiments to address both of these questions.

Citation

Bouchard LS, AO Sushkov, D Budker, JJ Ford, and AS Lipton. 2008. "Nuclear-Spin Relaxation of ^{207}Pb in Ferroelectric Powders." *Physical Review A* 77(2):022102 (6 pages).

Microstructures of ZnO Films Deposited on (0001) and *r*-cut α - Al_2O_3 Using Metal Organic Chemical Vapor Deposition

CM Wang^(a), LV Saraf^(a), and Y Qiang^(b)

(a) EMSL, Richland, Washington

(b) University of Idaho, Moscow, Idaho

Detailed knowledge of the structure of oxide thin films in relation to the substrate provides researchers important tools to enable the growth of films with the desired functional properties for specific applications. Such thin film studies further EMSL's goals to characterize surfaces and interfaces with unprecedented resolution as well as to design and synthesize increasingly complex materials.

Integrated deposition, diffraction, and microscopy resources housed at EMSL allowed researchers to study previously unknown structural details of oxide thin films that have potential applications to optoelectronics and spintronics. Earlier studies revealed differences in the qualities of zinc oxide (ZnO) films grown on different surfaces of crystalline Al_2O_3 – more commonly known as sapphire. EMSL users identified new and important microscopic details of the different ZnO thin film structures grown under identical conditions on Al_2O_3 surfaces with different crystalline orientations. Because thin film function depends on structure, such detailed characterization is a necessary step toward atomic-level design of thin films for targeted applications.

For their studies, the team from the Pacific Northwest National Laboratory and University of Idaho compared thin film growth on Al_2O_3 cut along two different planes to yield two different ZnO bonding surfaces, referred to as *c*-cut and *r*-cut. These Al_2O_3 surfaces consist of the same atoms, but for each cut the arrangement of the atoms is different. Under identical conditions, these bonding surfaces were used to grow ZnO thin films with EMSL's metal organic chemical vapor deposition capability. Differences in the ZnO thin films were then characterized using high-resolution transmission electron microscopy, electron diffraction, and high-resolution TEM image simulations. This research was featured in *Thin Solid Films*.

Citation

Wang CM, LV Saraf, and Y Qiang. 2008. "Microstructures of ZnO Films Deposited on (0001) and *r*-cut α - Al_2O_3 Using Metal Organic Chemical Vapor Deposition." *Thin Solid Films* doi 10.1016/j.tsf.2008.04.001.

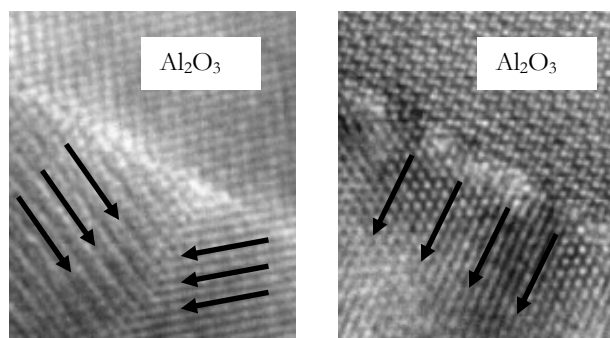


Figure 1. High-resolution TEM images of portions of ZnO thin films grown on *c*-cut Al_2O_3 (left) and *r*-cut Al_2O_3 (right). Arrows indicate the prime direction of the ZnO thin film. The *r*-cut substrate yielded high-quality single crystals.

Major Upgrades

Chinook. Phase II of EMSL's new supercomputer, Chinook, has been installed, and availability testing began in the fall.

Mossbauer Spectroscopy Laboratory. Upgrades to the Mossbauer Spectroscopy Laboratory included significant modernization of equipment and software to elevate the capability to current standards. Hardware upgrades included new computer systems with enhanced processing and storage capability as well as the necessary infrastructure to support them. In addition, networking capability and custom monitoring software that enables remote access were enhanced.

Rutherford Backscattering Spectrometry. Upgrades to the Rutherford Backscattering Spectrometry system resulted in replacement of antiquated hardware and optimization of system performance.

SPLAT Ruggedization. Efforts were completed to further ruggedize the Single Particle Laser Ablation Time-of-Flight Mass Spectrometer. The system is now better equipped to operate in harsh field conditions.

News Coverage

EMSL staff from the Instrument Development Laboratory and Computing and Networking Services were instrumental in a Department of Homeland Security project that culminated in testing of the system at the Toyota Center in Kennewick, Washington. The Tri-City Herald printed the following article:

Standoff explosives detection systems to be piloted at Toyota Center

PNNL is teaming with the U.S. Department of Homeland Security to test standoff explosives detection systems at the Toyota Center in Kennewick beginning Sept. 26.

For a series of six Tri-City Americans hockey games, a team of staff members from PNNL will field test infrared cameras and a millimeter wave radar probe as part of the Standoff Technology Integration and Demonstration Program pilot project.

Standoff refers to the distance between detection technologies and entrances to a large event such as an arena or coliseum. Rather than detecting explosives at an entrance, DHS would like to detect them such that the operators and the bulk of the public are outside of a potential blast zone. The multiyear program is focused on developing countermeasures for suicide bombers and vehicle-borne improvised explosive devices for national security or special events such as political conventions, sporting events, etc.

The field test includes exploring commercial off-the-shelf and near-commercial technologies that could be used simultaneously. Data from the field testing will be used by developers to adapt the technologies for inclusion in comprehensive security architectures.

The PNNL team will field test technologies to detect concealed objects such as suicide vests. High-powered imaging processing software will analyze surveillance camera images and look for anomalies such as abandoned bags, formation of groups, people loitering and more. Other surveillance cameras will be used to document the flow of people into the facility and to facilitate the interdiction process if the sensors detect a concealed object.

Nick Lombardo, National Security Directorate, is the project lead.

Awards and Recognition

Smith Named AVS Fellow. EMSL user Dick Smith—physics professor at Montana State University—was selected as a Fellow in the AVS: Science and Technology of Materials, Interfaces, and Processing. This not-for-profit society focuses on surface science, electronic and magnetic materials, nanoscience, and biomaterials. Smith received this honor for his outstanding expertise researching metal-metal interfaces. An award-winning researcher, Smith has more than 30 years of experience in investigating the structure and composition of metal-metal interfaces and studying the growth process as one metal is deposited on another. His work has been aided by the use of ion beam techniques, such as Rutherford backscattering and channeling instrumentation at EMSL.



Dick Smith

Lin Named Laboratory Fellow. Longtime EMSL user Yuehe Lin, of Pacific Northwest National Laboratory, has been named Laboratory Fellow, the highest rank that PNNL science and engineering staff can attain. Laboratory Fellows are chosen for establishing careers of sustained, highest-quality research and development in science or engineering fields. They are recommended by the Laboratory Fellow Review Committee, which has representation from across PNNL. Lin is a longtime contributor to the fields of chemical sensors and biosensors and biomedical nanotechnology. He and his co-workers have established a research program at PNNL for the development of nanomaterial-based chemical sensors and biosensors for environmental, homeland security, and biomedical applications. They have also developed functional nanomaterials for fuel cells, drug delivery, and environmental remediation applications. Lin has distinguished himself through his outstanding program development skills, his mentoring activities, and his publication excellence—he is frequently listed as author of highly cited papers and was recipient of the 2005 *Electrochemistry Communications* Award for the Best Cited Paper. He has more than 200 publications, including 20 invited book chapters, 166 journal articles, and 20 conference proceeding papers. He was recognized at a ceremony on August 6.



Yuehe Lin

Visitors and Users

During the fourth quarter of Fiscal Year 2008, a total of 340 users benefited from EMSL capabilities and expertise. This total included 255 onsite users and 85 remote users.

New EMSL Staff

Ray Teller joined EMSL on August 18 as the Associate Director for Scientific Resources. In his new position, Ray is responsible for oversight of EMSL's scientific capabilities and staff. He will help establish and guide strategies for revitalizing EMSL's capabilities, achieving EMSL's scientific vision, and bolstering user outreach. Ray previously served as Director of the Intense Pulsed Neutron Source, a DOE Office of Basic

Energy Sciences-funded national user facility at Argonne National Laboratory. At IPNS, he provided oversight of 90 staff and a \$17 million budget, and he established many partnerships and collaborations within the academic community, funding agencies, industrial partners, and other international and U.S. national laboratories.

Ping Yang joined the Molecular Science Computing Visualization group in August. She comes to EMSL from Los Alamos National Laboratory and will be a great asset to the consulting team as well as continuing research in actinide.

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

Publications

Book Chapter

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Conferences and Presentations

During the fourth 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:

- 6th International Conference on Photo-Excited Processes and Applications, Sapporo, Japan, on September 10, 2008.
- 8th Triennial Congress of the World Association of Theoretical and Computational Chemists, Sydney, Australia, September 15 – 17, 2008.
- 2008 DOE Summer School in Multiscale Mathematics and High Performance Computing, Richland, Washington, on August 5, 2008.
- 2008 Symposium of the Pacific Northwest Chapter of the American Vacuum Society, Richland, Washington, on September 18, 2008.
- Cyber-Enabled Instrumentation Strategic Planning Workshop CEI2008, Arlington, Virginia, on July 16 - 18, 2008.

- The Sixth Congress of the International Society for Theoretical Chemical Physics Vancouver, British Columbia, Canada on July 19, 2008.
- University of Kansas – Department of Pharmaceutical Chemistry, Lawrence, Kansas, on September 23, 2008.
- World Association of Theoretical and Computational Chemists Satellite Meeting, Takapuna, New Zealand on September 11, 2008.