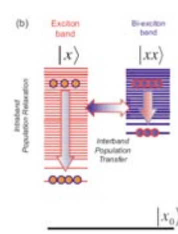
INDEX of SCIENCE HIGHLIGHTS   October 20, 2010



PADSTE HIGHLIGHTS October 20, 2010

AWARDS

Laboratory Distinguished Service Awards

Five individuals, five small teams, and seven large teams received 2009 Distinguished Performance Awards, a program that recognizes job performance above and beyond what is normally expected. The individuals and teams are described in the following paragraphs.

Individuals

Christopher S. Fugard (Nuclear Counterterrorism Response, IAT-3) added significantly to the National Nuclear Security Agency's (NNSA's) understanding of the technical issues shared by today's nuclear threats. His assessment of these emerging technologies, taking into account both their offensive capabilities and defensive measures that could be taken against them, has had an impact on NNSA's defense programs and its Nuclear Counterterrorism program.

Lorenzo Gonzales (Education and Postdoc Office, STBPO-EPDO) is a Master Teacher in the Northern New Mexico Math and Science Academy (MSA), LANL's community education outreach program for Northern New Mexico's K–12 teachers. He championed a Principals' Institute and an Ir-Rational Number Institute to give teachers additional mathematics instruction, initiated a new series of video teaching aids for MSA teachers, and supported a Laptop Initiative that introduced modern learning technologies and software into 39 MSA classrooms. Gonzales assisted Northern New Mexico College to implement a new Bachelor of Arts in Teaching program and to define a proposed new Master of Arts in Teaching Math and Science program. In addition, he was a key player in redesigning the University of New Mexico's Ed.D. in Educational Leadership program.

Jagdish C. (J.C.) Laul (Safety Basis Technical Services, SB-TS), a principal safety engineer, developed the technical bases that justified establishing lower hazard designations for six nuclear and nonnuclear Laboratory sites. He used his strong chemistry and nuclear background to provide a much better understanding of the actual risk each site poses. His work also establishes a valuable foundation of information for future remediation. Laul's characterizations and evaluations will reduce the cost of maintenance and surveillance at these sites, saving as much as $5 million a year.

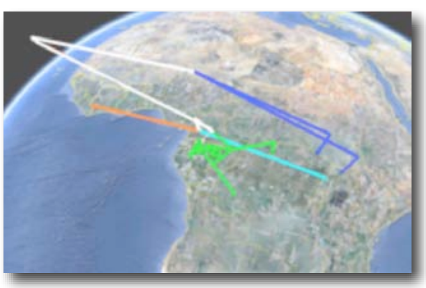
Howard J. Patton (Geophysics, EES-17) made scientific contributions in seismology and treaty verification. He developed and published a compelling and plausible theory to explain the unusual surface wave energy for the 2006 and 2009 North Korean tests. These tests had significant scientific challenges for identification because their surface wave energies were much higher than would have been expected for such explosions. His theory explains the unusual surface wave energy after the 2006 test, suggesting that explosions in virgin rock would generate significantly higher surface wave energy than in previously disturbed rock. He refined and validated his theory in analyzing the 2009 test. Surface wave discrimination techniques can now be adjusted to account for the energy increases in virgin rock explosions. His theory and mathematics could provide a transformational seismic-event identification capability for treaty verification, ensuring that virgin rock explosions will not be misidentified.

John E. Valencia (Space Science and Applications, ISR-1) is a driving force behind space programs supporting the nation's nuclear nonproliferation treaty monitoring capabilities. He was involved in work to complete production, testing, integration, and delivery of six combined X-ray spectrometer and particle dosimeter (CXD) payloads scheduled to fly on current-generation GPS IIF satellites. Valencia designed a substantially new and enhanced CXD sensor suite for the next generation of satellites, the GPS-IIIs. His work on the GPS-III sensors ensures that the Space Nuclear Detonation Detection program is well positioned for global coverage of nuclear threats during the next 20 years.

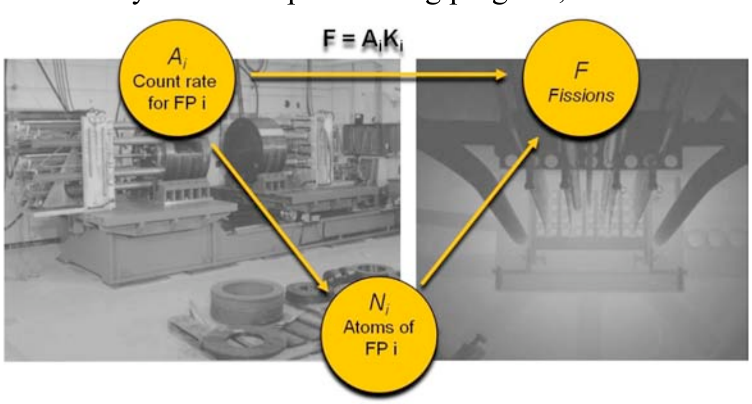
Small Teams

B83 Peer Review Team Lawrence Livermore National Laboratory (LLNL) asked Los Alamos to organize a peer review team and investigate a performance issue with its B83, a complex weapon with features not typically seen in Los Alamos designs. No weapon performance model for the B83 existed at LANL. In one year, the team developed a B83 full-system model, benchmarked it against a set of relevant nuclear test data, applied the model to the problem at hand, and rendered a technical judgment. Also, the team reviewed LLNL's work, compared its own results with LLNL results, identified and modeled other relevant nuclear tests, and provided further suggestions for changes LLNL could make in its technical work. The team's drive and determination to address a challenging physics problem faced by the laboratories when certifying the stockpile allowed them to complete a high-quality body of work in a short time. Scientists from X-Computational Physics and X-Theoretical Design divisions are W.R. Dearholt, D.F. Jablonski, J.A. Mercer-Smith, J.M. Scott, Y.-M. Wang, and R. Weaver.

Biodefense Informatics Team: As a result of the 2001 anthrax attacks, the Department of Homeland Security (DHS) manages a major effort to develop biodetection warning systems. To support DHS, the Biodefense Informatics Team developed a large set of validated assays to detect a variety of viral and bacterial biothreat organisms. Team members designed new assays and validated them experimentally against genetic material isolated from killed pathogens and closely related species, delivering nearly 80 assays to the DHS. The assays given to the Centers for Disease Control and Prevention (CDC) have added significantly to their repertoire of bioterrorism rapid response tools. The team provided LANL a new capability for assay validation that has led to follow-on efforts with the DHS. Team members from Bioscience and Theoretical divisions are N.A. Doggett, P.W. Fenimore, J.D. Gans, J. Song, C.J. Stubben, and M.A. Wolinsky.

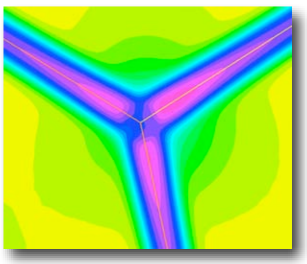


Fission Basis Team: Radiochemistry is a primary diagnostic method for analyzing debris in weapons tests. Early in the weapons testing program, radiochemists at LANL and Livermore used similar methods for the measurement and derivation of fissions, but later diverged in their approaches and in the data used for interpretation. This difference could inhibit the comparison of experiments between the laboratories and limit the ability to quantify uncertainties in radiochemical evaluations. Los Alamos worked with Livermore to resolve the differences by reexamining and documenting experimental work that formed the calibration basis for LANL's



measurement laboratory and then comparing these experiments with fission yields in the literature (primarily in plutonium). The accuracy of the Los Alamos data was verified, and an independent Livermore literature evaluation generated a set of fission chain yields much closer to those derived from LANL experiments. Reconciling the difference resulted in a consistent set of fission product data between the laboratories, a significant contribution to the weapons programs at both laboratories that resulted in a sound basis for assessing uncertainties in radiochemical interpretation. Participants from Chemistry, Computer, Computational, and Statistical Sciences, Information Resource Management, Theoretical, and X-Theoretical Design divisions are T.L. Graves, T. Kawano, A.L. Keksis, M.E. MacInnes, R.A. Meade, and H.D. Selby.

Multi-Scale Multi-Physics Modeling and Simulation for Nuclear Fuels Team: Future energy security will require a mix of energy sources, and nuclear energy will continue to make important contributions. This diverse team developed a framework for a multiscale, multiphysics modeling and simulation tool to predict nuclear fuel performance, supporting research into innovative fuel options. Developing new fuels is a long and expensive process. The basis for current fuel performance codes is empirical, requiring expensive irradiations and postirradiation examinations. Fuel performance codes are limited to the range of experimental data. The team created a framework with an atomistically informed mesoscale theory for metal and oxide fuels performance. This will enable scientists to replace empirically based fuel performance codes with "ab initio" based codes, a scientific breakthrough for the nuclear power field that should lead to extensive cost savings and increased material and performance flexibility. These technical contributions lay the foundation and underlying physics for a predictive fuel performance code, and LANL has been established as a leader in this field. Team members in Computer, Computational, and Statistical Sciences, and Materials Science and Technology divisions are D.R. Andersson, N.N. Carlson, P. Nerikar, C.R. Stanek, B.P. Uberuaga, and C. Unal.



ORCAS Hyperspectral Imager Team built and demonstrated an ultra-compact, low-power infrared imaging device, the Optimized Remote Chemical Analysis Spectrometer (ORCAS), in support of DOE's proliferation detection mission. Operating in the long-wave infrared (LWIR) wavelength, ORCAS can remotely detect chemical emissions from proliferant activities. For proliferation detection, DOE has long used LWIR hyperspectral chemical analysis of effluents, but until now LANL's role has been only to analyze data collected and donated by others. Los Alamos had no instrument program of its own. This team rectified that situation by building a deep understanding of issues limiting LWIR instruments and then developing a next-generation device that is suitable for deployment on unmanned aerial vehicles and is smaller, uses less power, and performs better than its predecessors. Two patents are now pending, and the ORCAS performance design and characterizations are being used worldwide. LANL's expertise and reputation in the field of infrared hyperspectral instrumentation has been raised to a newly competitive level. Researchers from Chemistry and International, Space and Response divisions are T.C. Hale, C.J. Hewitt, L.J. Jolin, Jr., and S.P. Love.

Large Teams

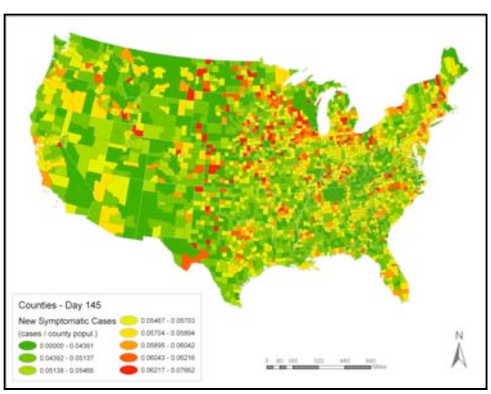
Algal Biofuels Consortium Development Team formed the National Alliance for Advanced Biofuels and Bioproducts (NAABB), a collaboration of scientists and engineers from companies, universities, and national laboratories, to address the challenge of alternative energy. The

NAABB
National Alliance For Advanced Biofuels and Bio-products

team was inspired by a collective vision for applying scientific and technical research on algae to meet the need for renewable fuels. The development team created a scientific strategy for algal fuels and secured $49 million in DOE funding, as well as $19 million in cost-share for the alliance to develop innovations for the algal biofuels industry. NAABB was the only biofuels consortium to receive such funding from DOE. This represents a major success for LANL, ensuring recognition for its contribution to a broad national security mission. Team members from Biosciences, Chemistry, Chief Financial Officer, Earth and Environmental Sciences, Engineering and Engineering Sciences, Information Resource Management, Laboratory Counsel, and Technology Transfer are A. Abdel-Fattah, C. Carmer, B. Cottrell, R. Currier, D. Fox, G. Goddard, C. Gomez, D. Hadley, J. Heikoop, A.T. Koppisch, L. Martinez, R. McDonald, M. Morgan, D. Newell, J. Olivares, M. Park, D.R. Pesiri, D.J. Salazar, L. Silks, III, E. Sullivan, S. Twary, C. Unkefer, P. Unkefer, and C. Zerkle.

Fall Classic Project Team planned and executed a 6-week campaign at the Nevada Test Site to test and validate tools and techniques for nuclear diagnostics and modeling. The campaign involved more than 200 U.S. and international participants from the scientific and emergency response communities. During the exercise, emergency responders tested their skills, equipment, and procedures. Scientists made benchmark measurements and collected nondestructive assay data that will be used to validate new equipment, refine software analysis techniques, and develop procedures fundamental to understanding and responding to nuclear threats. LANL team members made these accomplishments possible by obtaining all the safety, security, and operational approvals while coordinating the myriad technical, logistical, and administrative details with other agencies and laboratories. The Fall Classic enhanced the ability of the U.S. and its allies to recognize and respond to a wide variety of nuclear threats. Participants from International and Applied Technology, Global Security, Joint Nevada Program Office, Nuclear Nonproliferation, Operations Support, Physical Security, Plutonium Manufacturing and Technology, Prototype Fabrication, Quality Assurance, Radiation Protection, Safety Basis, Weapons Programs, Weapon Systems Engineering, and X-Computational Physics are J. Bounds, D. Bourcier, D. Bowen, D. Carlisle, J. Carpenter, R. Castro, L. Champ, R. Chrien, S. Clement, D. Dinwiddie, A. Downs, T. Dugan, J. Dyson, S. Fellows, S. Garner, S. Gonzales, W. Haag, R. Hammer, C. Harmon, S. Hoover, R. Kasik, S. Keller, J. Koster, K. Lacy, D.K. Lash, G. Macleod, E. Martinez, M.Y. Martinez, Y. Martinez, F. Martinez, Jr., S. Monahan, W.Myers, J. Paisner, T. Pollat, E. Rose, R. Roybal, M. Salazar, K. Scott, E. Shores, M. Smith-Nelson, A. Sood, G. Sundby, G. Torres, S. Traeger, L. Trujillo, L. Ussery, K.E. Valdez, F.J. Valenzuela, E. Vest, M.A. Vigil, M. Weaver, and T. White.

H1N1 Analysis Team: LANL's National Infrastructure Simulation and Analysis Center (NISAC) performed a study of the risk of an H1N1 pandemic, running simulations before an anticipated reappearance in the fall of 2009. The scientists simulated the potential spread of H1N1 across the globe and through the U.S. and 214 other countries. The team evaluated medical supply logistics and the impacts of closing schools, restricting travel, encouraging self-isolation, and using antiviral drugs, vaccines, and protective masks. They used models of the U.S. health care system to evaluate the pandemic's impact on hospital capacity, and they estimated workforce absenteeism and risk for the Department of Homeland Security (DHS). Developing predictive, quantitative analyses to anticipate



the consequences of disruptions to critical infrastructure and resources is fundamental to the Lab's mission. DHS recognizes the H1N1 Analysis Team as the authoritative analysis source for H1N1 impacts. Scientists from Bioscience, Computer, Computational, and Statistical Sciences, Decision Applications, Information Resource Management, and Theoretical are J. Ambrosiano, R. Bent, L. Dauelsberg, S. del Valle, B. Edwards, J. Fair, S. Flaim, T. Germann, L. Inkret, R. Leclaire, Jr., S. Linger, B. McMahon, S. Mniszewski, L. Moore, F. Pan, D.R. Powell, M.K. Rivera, and P. Stroud.

LANL MATLS-PE-09 Proficiency Test Team was a highly successful participant in a national nuclear forensic test aimed at developing national capabilities for identifying and analyzing interdicted special nuclear materials. Each participating team received a unique, unidentified actinide material to analyze. The LANL team was the only participant to complete and report all required measurements, including 61 elemental, 15 isotopic, and 1 chronometric. The team met all deliverables on time, within 12 working days, and achieved the best accuracy and precision. The MATLS-PE-09 Proficiency Test Team demonstrated that LANL expertise and experience are the nation's best for interdicted special nuclear material analysis. Team members from Bioscience, Chemistry, Chemistry and Metallurgy Research, Nuclear Nonproliferation, Radiation Protection, and Waste and Environmental Services are: A. Aragon, G. Bland, W. Chroninger, L. Colletti, M.J. De La Torre Garcia, S. Dempsey, K. Duran-Suazo, J. Dyke, K. Espinosa, J. Fulwyler, D. Gallimore, K. Garduno, A. Gomez, M. Gubernatis, T. Hahn, D. Hobart, R. Keller, K. Kuhn, K. Laintz, D. Lanford, E. Lujan, S, Maestas, F. Martin, A. Martinez, D.J. Martinez, P.T. Martinez, P. Mendoza, S. Myers, J. Miller, D. Peterson, D. Porterfield, C. Riebe, J. Rodriguez, W. Sandoval, C. Soderberg, K. Spencer, L. Tandon, M. Thomas, R. Torrez, L. Townsend, J. Trujillo, A. Valdez, J. Valdez, G. Valentine, G. Vuyisich, L. Walker, A. Wong, C. Worley, N. Xu, and C. Zocco.

NCam Airborne Deployment Team successfully demonstrated the utility of its novel NCam single-photon imager for collecting data relevant to DOE's nonproliferation mission. Team members planned, implemented, integrated, mounted, and analyzed an airborne experimental campaign to demonstrate their technology on a NASA aircraft entirely new to them and completed their work in only four months. This effort involved extremely long hours and many weeks at multiple locations for integration, engineering flight tests, and the experimental flight campaign. Members worked under difficult field conditions, building and deploying ground targets and performing ground-truth measurements. The result was the first system NASA aircraft operators had ever seen deployed on their aircraft that worked immediately upon installation. The team's high level of scientific and technical expertise, along with its ability to work under stress, has drawn continued interest from other agencies impressed by the team's growing reputation for bringing in difficult projects in relatively short times. Team members from Accelerator Operations and Technology, Chemistry, High Performance Computing, International, Space and Response divisions are S. Buck, L. Chavez, R. Des Georges, S. Greenfield, G. Lujan, B. McVey, J. Mondragon, P. Montano, I. Owens, D. Palmer, D. Remelius, R. Shirey, L. Stonehill, D.C. Thompson, J. Tiee, M. Ulibarri, R. Whitaker, and S. Whittemore.

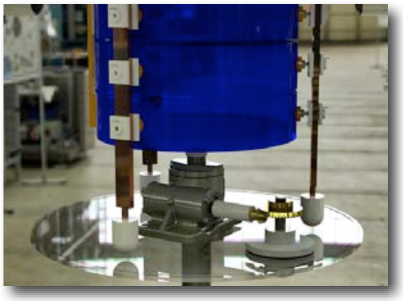
NISC SCIF Expansion Project Team: Expansion of the Sensitive Compartmented-Information Facility (SCIF) in the Nonproliferation and International Security Center (NISC) was critical for preserving and enhancing LANL's technical resources and capabilities to handle sensitive compartmented information and to support our global security and nuclear weapons defense national security missions. The team was responsible for converting the third floor of the fully occupied

building—where numerous secure computers are operated and classified documents are routinely reviewed—to a SCIF. This required significant oversight and coordination of construction activities in a highly secure facility, while several hundred employees in the building continued to perform critical programmatic activities. The construction phase was completed within a compressed time frame and fixed budget. LANL can more effectively address its national security missions now and in the future. Team members from Chief Financial Officer, Construction Management, Cost, Schedule and Estimating, Engineering Services, Field Intelligence Element, Industrial Hygiene and Safety, Infrastructure Planning, International and Applied Technology, International, Space and Response, Maintenance and Site Services, Network and Infrastructure Engineering, Nuclear Nonproliferation, Office of Counterintelligence, Physical Security, Project Management Function, Quality Assurance, Science and Technology Operations, and Security Operations are M.W. Adkins, T. Ball, H. Barela, P. Blumberg, J. Bonn, M. Carlson, D. Carr, D. Chastain, S. Cisneros, J. Crook, G.R. Delgado, R. Epperson, C. Finn, A. Gallegos, E.S. Garcia, L. Garcia, W. Gonzales, M. Haber, R. Hammer, B. Herrera, P. Hudson, R. Kierstead, J. Leeches, D. Lichliter, S. Littleton, R. Logan, G. Lopez, F. Lujan, D. Maez, A. Marquez, S. Marriott, A. Martinez, Jr., G. McFarlane, D. Lowe, A. Morrison, S. Parks, J. Parrack, Jr., D. Pompeo, J. Privette, Z. Robinson, K. Rose, M. Roybal, J. Rudnick, S. Strain, P. Tripplehorn, M. Turner, D. Tyson, G. Velasquez, H. Villareal, G. Winsemius, II, and L. Yost.

Small Sample Plutonium Machining Team: A successful weapons program depends upon the fabrication of complex plutonium test samples and parts that are essential for subcritical experiments, small-scale assessment tests, and National Ignition Facility targets. These fabricated pieces are fundamental for qualification and recertification of the stockpile. Historically, Stockpile Manufacturing and Support was able to meet a small subset of requests because of insufficient machining resources, capability, and capacity. The team embarked on a process/capital improvement project to establish a viable sample-fabrication program and created a state-of-the-art machining laboratory that now produces test specimens previously considered too difficult to fabricate. During active construction of the site, more than 160 components were fabricated for the national security complex. No parts were scrapped, and scheduling and quality requirements were exceeded for all projects. The program now sets the standards for technology development and transfer, and members are recognized as "the experts" in the nuclear weapons complex for fabricating complex plutonium components. Team members from Applied Engineering and Technology, Cost, Schedule and Estimating, Engineering Services, International and Applied Technology, International, Space and Response, Maintenance and Site Services, Materials Science and Technology, Plutonium Manufacturing and Technology, Prototype Fabrication, Radiation Protection, Quality Assurance, Safety Basis, Stockpile Manufacturing and Support, Weapons Component Manufacturing, Weapons Systems Engineering, and X-Theoretical Design are R. Allen, A. Archuleta, B. Art, K. Art, F. Bailon, T. Baros, E. Blue, W. Blumenthal, S. Boggs, T. Bradshaw, W. Brown, W. Cantrell, H. Chacon, A. Chavez, D. Chavez, D. Conger, G. Cornejo, D. Dennison, P.A. Duran, K, Fisher, F. Freibert, A. Gabaldon, D. Gallant, G. Gallegos, J.J. Gallegos, V. Griego, F. Hampel, D. Haring, C. Harmon, D. Huerta, L. Jaramillo, C. Larribas, M. Lavigne, S. Lieberwirth, R.J. Lopez, J. Lugo, E. Martinez, J.P. Martinez, K.R. Martinez, S.D. McKee, Mirko Mikan, T. Milligan, C.M. Montoya, E. Montoya, P.M. Montoya, S. Ney, R. Olivas, R. Ortega, U.I. Page, J.L. Parker, M. Prime, M. Probasco, L. Quintana, M. Rainbolt, M. Ramos, Y. Rivera, W. Robertson, P. Rodriguez, J.P.M. Romero, R.D. Romero, A. Ross, J. Rubin, J. Rutten, T. Saleh, W. Santistevan, L. Shay, R. Simpson, W. Smith, S.M. Sterbenz, B. Storey, R. Suazo, D. Thacker, M.T. Trujillo, J.A. Valdez, and A. Van Etten.

APPLIED ENGINEERING TECHNOLOGY

Glovebox penetration-free mold lift for TA-55 PF-4 foundry



Members of Process Control & Automation Group (AET-5) engaged the Colorado School of Mines (CSM) to develop a prototype replacement for the mold lift in the plutonium foundry. As a Senior Design Project last school year, CSM developed a design that included a non-lubricated jack screw driven by a motor through a unique magnetic coupling. The magnetic coupling transmits rotation of the lift through the glovebox floor without penetrating the glovebox wall.

Photo: CSM lift design with drive coupled through the glovebox floor.

This summer, AET-5 gave Nicholas Kutac, a senior in mechanical engineering from New Mexico State University, the assignment to design and build the next evolution of this prototype. The prototype uses a cup-shaped magnetic coupling in a linear arrangement. Kutac assisted with design and performed stress analysis, which yielded design improvements to include a lower bearing and an increase in rod diameters. The TA-50 Prototype Fabrication Shop, with oversight from Abe Chavez (Fabrication Services, PF-FS), fabricated the parts. The internal assembly is complete, and the prototype housing is being finalized. The design had many bearing surfaces that require precise machining to tight tolerances. The parts went together perfectly following fabrication in Chavez's shop. The lift will be coupled through a fixed stainless steel barrier to the drive motor outside of the glovebox. This new lift design will undergo extensive testing before the units that will be used in TA-55 PF4 are fabricated. The Plutonium Sustainment Maintenance Program in Stockpile Manufacturing and Support (ADSMS), (Howard Granzow, LANL Program Manager), supported the work.

Photo: Nicholas Kutac holding internal lift assembly with PF-FS lead Abe Chavez.

BIOSCIENCE

How human pathogens attack the immune system

Human pathogens have evolved sophisticated mechanisms by which to attack the host immune system. One such mechanism is the Type III secretion system (TTSS), a "syringe-like" needle complex that injects virulence proteins, or effector proteins, into the host cell. Elizabeth Hong-Geller, Kristy Nowak-Lovato, Sofiya Micheva-Viteva, and Sabine Lauer (Biosecurity and Public Health, B-7) were invited to write a book chapter "Regulation of Host Chemokine Response by the Pathogenic Type III Secretion System" in the volume ***Chemokines: Types, Functions, and Structural Characteristics*** (Nova Science Publishers, in press). The chapter describes pathogen effector interactions with multiple host protein targets to modulate the host inflammatory response, enabling pathogen survival and colonization of the host. TTSSs have been found in over a dozen Gram-negative animal and plant pathogens, underscoring the conservation of this virulence mechanism as an effective strategy for host infection. In the host, chemokines, or chemotactic cytokines, have emerged as central regulatory molecules, forming chemoattractant gradients that direct the migration of neutrophils and macrophages to sites of infection.

In multiple studies, chemokine mRNA and protein expression levels have been shown to be regulated in response to host infection by TTSS pathogens, implicating TTSS effector proteins in the activation of chemokine function. This review details the molecular mechanisms by which TTSS effector proteins modulate chemokine function in the host and focuses on the TTSSs from three potential agents of bioterrorism: the CDC Category A pathogen *Yersinia pestis* and the Category B pathogens, *Burkholderia pseudomallei* and *Salmonella typhimurium*, the causative agents of plague, melioidosis, and gastrointestinal disease, respectively. Study of host immune responses to TTSS effector proteins will provide mechanistic insights into the TTSS infection strategies used by other high-risk pathogens. Elucidation of TTSS virulence mechanisms may serve as the basis for design of novel inhibitor therapeutics that block TTSS-based pathogen infection. LANL Laboratory Directed Research and Development (LDRD) funded the writing of this review.

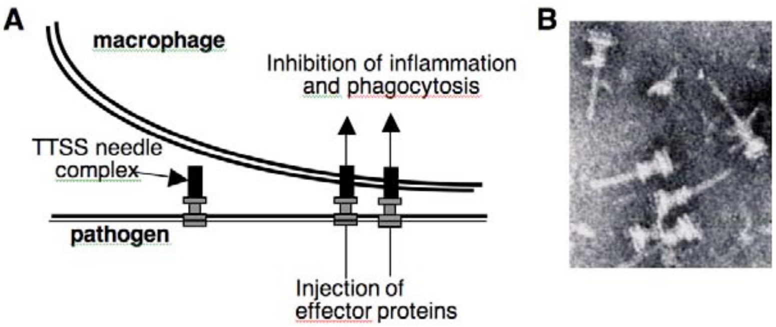


Figure 1. (*A*) Schematic of pathogen effector transport via TTSS into macrophage; (*B*) Electron micrograph of purified *Salmonella typhimurium* TTSS (***Microbes Infect*** 2002, *4*: 75)

CHEMISTRY

ENABLE technology creates high-aspect-ratio etched structures for cancer screening

The ENABLE (Energetic Neutral Atom Beam Lithography & Epitaxy) team is working with Creatv MicroTech, Inc. through a CRADA agreement to create high-aspect-ratio structures for a number of applications. ENABLE employs an energetic, reactive, and collimated beam of neutral oxygen or nitrogen atoms as the active etching species. It comprises a dual-function nanofabrication technology capable of both etching high-aspect-ratio nanostructures and growing thin films of semiconducting and superconducting materials. The technology can etch nanoscale structures into any material able to form a volatile product with oxygen, such as hydrocarbon polymers, graphite, etc.

The collaborative work with Creatv MicroTech is funded through the National Institutes of Health, and it focuses on creating improved X-ray anti-scatter grids to enhance the image quality of digital mammography systems. These improved grids are fabricated by first etching large scale arrays of approximately 60 x 60 micron square pillars that are about 250 micron tall spaced a few micrometers apart for some applications, and arrays with smaller pillars only 20 x 20 microns about 125 micron tall. After ENABLE etches these high aspect ratio structures, the template pattern is backfilled with a high-density metal by electroforming. Currently, the ENABLE technology is able to process a 5 cm diameter area and has produced prototype grid arrays that are about 1 x 1 cm in size. The ENABLE technology is being scaled up to a 24 x 30 cm platform, the size needed for anti-scatter X-ray grids on commercial systems. Currently, the X-ray anti-scatter grid needs to be moved during image acquisition to avoid the grid shadow in the mammography image. The goal of this collaborative LANL/ Creatv MicroTech project is to use ENABLE to produce X-ray grids for digital mammography that would not need to be moved during image acquisition. The target date for delivering a scaled up grid is September 2011. Mark Hoffbauer, Todd Williamson, and Jonathan Hubbard (Chemical Diagnostics and Engineering, C-CDE) comprise the ENABLE team. Technical contact: *Todd Williamson*

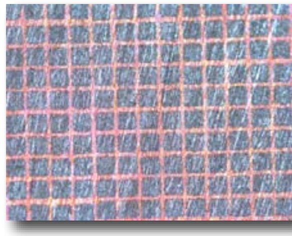


Figure 2. Clean etching of 250-micron thick polyester film with 7-8 micron wide trenches and 65-micron periodicity. Following etching, copper is electroformed into the trenches to make the X-ray anti-scatter grid.

LANSCE

LANSCE-NS Hosts NNSA Academic Alliance Center of Excellence Leader

Professor Jolie Cizewski of Rutgers University is on sabbatical as a Visiting Scholar and working with Neutron and Nuclear Science (LANSCE-NS) staff through December. Cizewski, who began her career as a postdoctoral researcher at Los Alamos in 1978-80, is the leader of an NNSA Stewardship Science Academic Alliance Center of Excellence. Cizewski's work focuses on understanding neutron capture reactions and developing alternative experimental and theoretical techniques to determine neutron capture reaction rates where direct measurements are difficult or not possible. Knowing these reaction rates, particularly for small and unstable samples, is important in understanding past nuclear weapons tests as well as understanding the creation of elements in stars. She is leading an experiment at LANSCE using high-resolution gamma-ray detectors to gain insight into spin distributions following neutron capture. These data, compared to data obtained with alternate reactions that probe the same nucleus, will allow evaluation of the accuracy of alternate reaction techniques. Several postdoctoral researchers and students are participating in the experiment in collaboration with Cizewski and LANSCE-NS staff.

Photo: Professor Jolie Cizewski (front center) with collaborator Bill Peters and postdocs Meredith Howard and Remi Adekola.

MATERIALS PHYSICS AND APPLICATIONS

Magnetism and electricity couple in a new organic material

Scientists from the National High Magnetic Field Laboratory, in collaboration with researchers from the Paul Scherrer Institute and the University of Maryland, have discovered a new class of materials. In research appearing as an editor's suggestion in ***Physical Review B***, the researchers report on multiferroic behavior in an organometallic compound containing magnetic copper ions in a lattice of methyl groups.

Magnetoelectric multiferroics are compounds with magnetic and electric orders that coexist and are coupled via magnetoelectric interactions. Research is motivated by the promise of devices that can sense and create magnetic polarizations using electric fields and vice versa, thereby creating new functionality as well as improving the speed, energy efficiency, and size of existing circuits. Most magnetoelectrics and multiferroics are transition metal oxides or fluorides where the magnetoelectric interactions are mediated via superexchange through the oxide and fluoride anions.

Vivien Zapf, Fedor Balakirev, and Frederik Wolff-Fabris (Condensed Matter and Magnet Science, MPA-CMMS), and collaborators M. Kenzelmann (Paul Scherrer Institute, Switzerland) and Y. Chen (University of Maryland) examined field-induced multiferroic behavior in an organometallic quantum magnet, copper dimethyl sulfoxide dichloride (CDC) containing S=1/2 Cu spins. The fast-pulsed magnetic fields at the National High Magnetic Field Laboratory allowed researchers to probe this coupling between magnetism and electric polarization with unprecedented sensitivity. Competing, frustrated magnetic interactions cause the copper spins to order in a complex non-coplanar structure that breaks a key symmetry (spatial inversion symmetry), creating a unique axis in the crystal. This allows an electric polarization to form. The CDC undergoes a magnetoelectric quantum phase transition where both ferroelectric and magnetic order emerge simultaneously as a function of magnetic field at very low temperatures. Thus, the magnetism and electric polarization are closely coupled. Because the magnetic order in CDC is mediated by large organic molecules, magnetoelectric interactions can exist in this important class of materials, opening the means to design magnetoelectrics and multiferroics using large molecules as building blocks. This finding creates the opportunity towards molecule-based designer magnets based on a wider range of organic ligands, in which desired magnetoelectric properties could be fine-tuned. Reference: "Magnetically induced electric polarization in an organometallic magnet," ***Physical Review B Rapid Communications***, 82, 060402(R) (2010); doi: 10.1103/PhysRevB.82.060402. The LANL Laboratory Directed Research and Development (LDRD) program, the National Science Foundation, and the National High Magnetic Field Laboratory funded various aspects of the research. Technical contact: *Vivien Zapf*

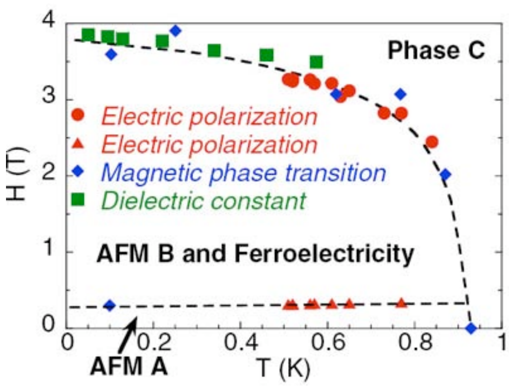


Figure 3. Phase diagram of CDC showing regions of antiferromagnetism (AFM) and ferroelectricity as a function of magnetic field H and temperature T.

MATERIALS SCIENCE AND TECHNOLOGY

A polycrystalline scintillator for nuclear material detection

Scintillators, materials that glow when struck by high-energy particles or photons, are used in radiation detection. Efficient, readily fabricated scintillators are needed for detection and verification of shielded special nuclear material at our nation's ports of entry and for use in large panels for radiation monitoring along our unattended air, land, and sea borders. A scintillator with high optical transparency is required for the transmission of the scintillating light to the photon detector. Transparent polycrystalline ceramics require a cubic structure in order to have the same refractive index along all crystallographic axes. Current state-of-the art polycrystalline scintillators ($LaBr_3$:Ce and $LaCl_3$:Ce) have a hexagonal structure, which is noncubic. Therefore, these scintillators cannot achieve true optical transparency unless a single crystal, a grain texturing, or a nanosized grain structure is formed. Fabricating the scintillators to these physical requirements is expensive and logistically difficult due to their oxygen and moisture sensitivity.

Ching-Fong Chen and Heather M. Volz (Materials Technology: Metallurgy, MST-6) and collaborators from MER Corporation and Sandia National Laboratories have developed a different type of transparent polycrystalline scintillator, an oxide ceramic. Their goal was to create a cerium-doped spinel

($MgAl_2O_4$:Ce), which can be fabricated using existing ceramic forming techniques of hot-pressing powder. These techniques can produce materials in large quantities, in large sizes, at fast rates, at low cost, and in net-shape. The resulting oxide ceramics have high mechanical strength, good stability in air and moisture, and high sinterability.

$MgAl_2O_4$ has great potential as a transparent scintillator material due to its good optical properties and stability in moisture and air. Its mechanical properties are comparable with polycrystalline aluminum oxide, and it has a cubic structure (i.e., no birefringence). Polycrystalline spinel can transmit light from 200 to 5500 nm with no optical distortion. Although $MgAl_2O_4$ has a lower stopping power for gamma rays compared with $LaBr_3$:Ce or $LaCl_3$:Ce, this problem could be easily overcome by increasing the thickness of the scintillator material.

The scientists addressed the means of fabricating a transparent polycrystalline $MgAl_2O_4$ scintillator using the correct dopant and optimized processing conditions. Because of its promising scintillation properties, the scientists used cerium (Ce) as the dopant and lithium fluoride (LiF) as a sintering aid to achieve a fully dense structure of $MgAl_2O_4$:Ce. The researchers demonstrated the feasibility of using a hot-pressing technique to make a transparent $MgAl_2O_4$:Ce polycrystalline single phase ceramic from powders. A perfectly polished spinel has a transmission of about 88% for 3-micron light. A polished 2-mm thick sample of the fabricated $MgAl_2O_4$:Ce has a high infrared (IR) in-line transmission of approximately 86%, a 50% transmission within the visible range, and about 40% at the excitation peak of 410 nm. The scientists suggest that the reduced light transmission for visible and ultraviolet light is due to light scattering off small residual pores on the order of about 1 micron. Reference: "Characterizations of a Hot-Pressed Polycrystalline Spinel:Ce Scintillator", ***Journal of the American Ceramics Society*** *93*, 2399 (2010); doi: 10.1111/j.1551-2916.2010.03721.x. The research supports LANL's global security mission area. The Nuclear Nonproliferation Office (Nancy Jo Nicholas, LANL Program Director) supported the work at LANL. Technical contact: *Chris Chen*

Photo: A polished $MgAl_2O_4$:Ce sample with 2-mm thickness. The polished disk was raised using six U.S. quarters, a distance of approximately 10 mm, to demonstrate its true transparency. The sample was highly transparent, and lettering can be clearly read through it. For most of the translucent ceramics, the transparency disappears when the sample is raised to 10 mm.

PHYSICS

Future home of MiniCLEAN appears in *Physics Today*

A number of observations have shown that over 20% of the universe is composed of "dark" matter, which does not interact electromagnetically. A variety of theoretical particles have been proposed that could account for dark matter, but no direct observation has been made. The MiniCLEAN detector is a LANL-lead experiment that uses liquid argon as the dark matter recoil target in the search for Weakly Interacting Massive Particles (WIMPs), a proposed dark matter candidate particle. MiniCLEAN utilizes a spherical geometry to maximize the light yield using cold photomultiplier tubes in a single-phase detector. Pulse shape discrimination techniques separate nuclear recoil signals from electron recoil backgrounds. ***Physics Today*** [Sept, 2010, pg 25-27] highlighted SNOLAB (an underground science laboratory specializing in neutrino and dark matter physics) and future location of MiniCLEAN in an article lauding the international renaissance in deep underground experimental facilities. The article describes the science and facility supporting MiniCLEAN, and the progress constructing the MiniCLEAN vessel in anticipation of its coming online deep underground at SNOLAB in Sudbury, Canada next year. LANL Laboratory Directed Research and Development (LDRD) funds MiniCLEAN, which is part of the international CLEAN/DEAP collaboration pursuing a staged approach to WIMP detection. Technical contact: *Andrew Hime*

Photos: (*Left*) Image excerpted from ***Physics Today*** [Sept, 2010, pg 26]: "The deepest underground lab for now is the recently completed SNOLAB in Canada. One of several new experimental halls will host two dark-matter search experiments that are set to be installed in the next two years." The opening on the right will house the LANL Neutron Science and Technology (P-23) dark matter search experiment MiniCLEAN. (*Right*) MiniCLEAN Inner Vessel hemispheres leaving LANL on their way to Winchester Precision Technologies for machining and welding.

THEORETICAL

Exciton scattering model for carrier multiplication in semiconductor nanocrystals

Recent work to develop new photovoltaic devices has addressed the problem of carrier multiplication in semiconductor nanocrystals. Carrier multiplication generates more than one electron-hole pair per single absorbed photon. The ability to produce two or more carriers instead of one per single absorbed photon can lead to dramatic increases in the efficiency of photovoltaic devices. Experimental studies of carrier multiplication in nanocrystals raise an important question of what specific quantum-confinement-induced features determine the quantum efficiency.

Andrei Piryatinski and Kirill Velizhanin (Physics of Condensed Matter and Complex Systems, T-4) propose a general theoretical approach capable of treating the carrier multiplication dynamics in both nanocrystals and bulk by accounting for a variety of key processes on the same footing. They achieve this by integrating the scattering theory with the density matrix formalism. The researchers call this approach the Exciton Scattering Model. They demonstrate that the previously proposed models can be recovered as limiting cases. The scientists show that the proposed model predicts additional pathways of carrier multiplication not considered before. They use the Exciton Scattering Model to formulate a closed computational scheme for numerical simulations of the carrier multiplication dynamics in nanocrystals and in bulk. Their work sets the stage for clarification of the quantum-confinement effect on the quantum efficiency. Reference: “An Exciton Scattering Model for Carrier Multiplication in Semiconductor Nanocrystals: Theory”, ***Journal of Chemical Physics*** *133*, 084508 (2010); doi:10.1063/1.3474576. LANL Laboratory Directed Research and Development (LDRD) and DOE Office of Basic Energy Sciences funded different aspects of the research.

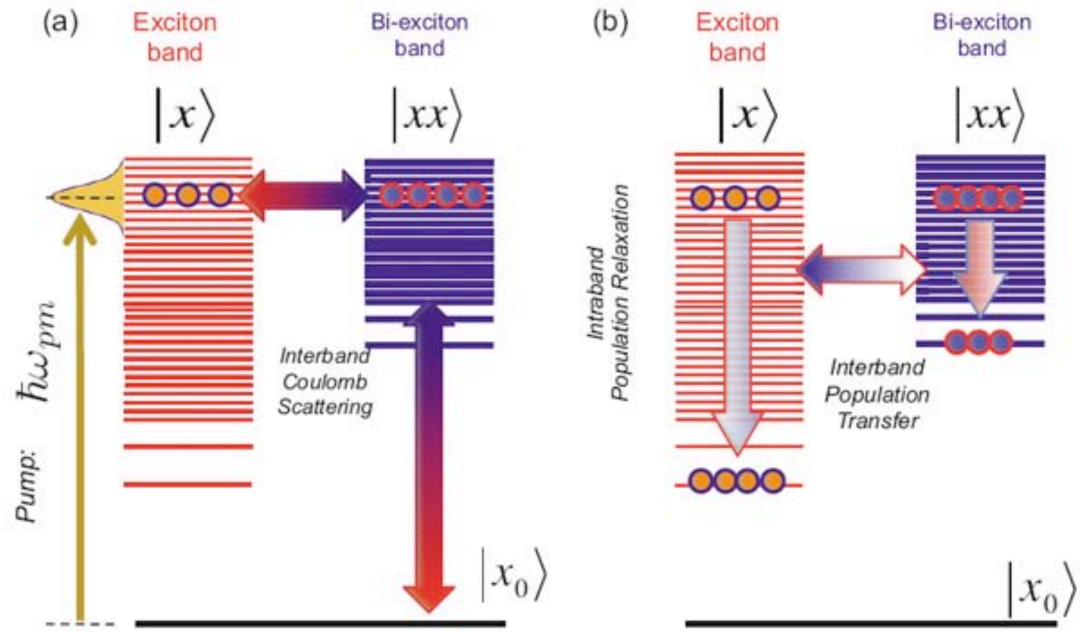


Figure 4. Level diagram of carrier multiplication dynamics in an ensemble of nanocrystals. (a) Photoexcitation by a pump pulse with central frequency ω_{pm} and finite spectral widths results in the generation of single- and biexciton populations in which the Coulomb scattering mixes all interband and intraband dipole transitions present. (b) During the population relaxation, both the intraband and the interband processes are mixtures of the phonon-assisted processes and Coulomb scattering events.