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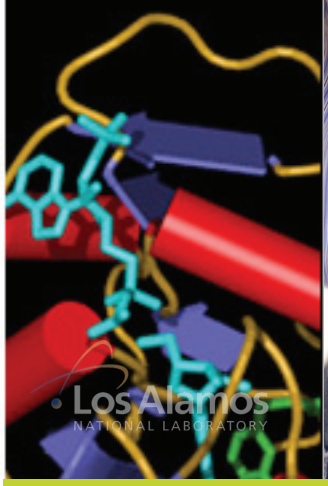

Fredrik Tovesson

On track to a better understanding of nuclear fission

By Francisco Ojeda
ADEPS Communications

As a physics graduate student at Sweden's Örebro University, Fredrik Tovesson became captivated by what happens when the nucleus of an atom splits. At a time of great scientific discussion about the construction of accelerator-driven nuclear reactors, he undertook the challenge to learn more about nuclear fission.

"I find nuclear fission fascinating because of the many open questions about this complex process, even though it was first discovered more than 70 years ago," said Tovesson, of Nuclear Science (LANSCE-NS). "By developing a better understanding of fission we can also better predict behavior in nuclear devices, reactors, and even astrophysical events."

Tovesson leads the Los Alamos effort on the Time Projection Chamber. The project, a collaboration between three national laboratories and six universities, is designed to allow the first-ever three-dimensional visualization of nuclear fission events. A prototype chamber has been installed and is being tested at the Weapons Neutron Research (WNR) facility at the Los Alamos Neutron Science Center.

The Time Projection Chamber is part of the Neutron Induced Fission Fragment Tracking Experiment, which through the more exact study of nuclear fission hopes to aid in the construction of safer, more efficient, and less waste-producing nuclear reactors.

"The next generation of nuclear reactors will use different technology than the current fleet, and there is a need for more accurate nuclear data to support this effort," Tovesson said. "Also, defense-related technologies such as nuclear forensics rely on accurate nuclear data to make reliable decisions on nuclear events after the fact."

Far superior to other detectors used for fission research, the Time Projection Chamber measures fission cross sections of the major actinides to better than 1% precision over a wide incident neutron

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From Alex's Desk

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Colleagues,

This is my first note from LANSCE's DO Desk. First, let me tell you how excited I am at being the selected candidate for the LANSCE Deputy Division Leader job. The level of activities, the size of the user programs, the scientific diversity—and lets not forget—the complexity at all levels makes this job very exciting. And just so you know, I am one of those that strives for complexities and appreciates and celebrates small victories and accomplishments. So, great job indeed.

'This is a great time for the LANSCE mesa.'

This is a great time for the LANSCE mesa. You have probably heard of the D'Agostino (Under Secretary for Nuclear Security), Johnson (Under Secretary for Energy) and Koonin (Under Secretary for Science) letter to the LANL Director about LANSCE. To my knowledge, this is the first time the Under Secretaries co-signed a letter with such high praise and support for LANSCE. The letter specifically mentions LANSCE's past and current role to NNSA's missions as well as to DOE Basic Energy Sciences. The letter also requests a plan for an enhanced maintenance program for the LANSCE facility. In addition, a clear reference is made regarding the Department's interest in materials under extreme conditions relevant to fission, fusion, and weapons systems.

We have contributed considerably to the Director's response to the three Under Secretaries' letter. LANL's response included a detailed LANSCE - LINAC investment plan and the Institution plans for MaRIE. It is important to notice that the MaRIE project that brings together the F^3 (Fission Fusion materials Facility), M4 (Making, Measuring, and Modeling Materials Facility) and MPDH (Multi-Probe Diagnostic Hall) facilities will be all co-located at TA-53 where the LANSCE accelerator will play a paramount role. And remember, we have an exercise room, and a cafeteria on site..... honestly folks, life can't get better than that.

We have also received authorization and funding from the LANS Board of Governors to build a new experimental building that will considerably increase LANSCE's ability to host more industrial users and better serve the Weapons Program.

And, I must add, two weeks ago when Kurt Schoenberg, John Sarrao, and I were visiting the CEA (Commissariat a l'Energie Atomique) in Bruyeres-le-Chatel, France we got a very pleasant surprise. The Scientific Director in his overall CEA talk described with great detail the current collaboration with LANSCE and its growth potential. In fact, its most recent Annual Activity Report features a picture of FIGARO (Fast Neutron-Induced Gamma-Ray Observer at LANSCE-NS) right on the cover pages. Also important to mention is the successful commissioning of the prototype TPC (Time Projection Chamber) by Tovesson et al. (LANSCE-NS), Lawrence Livermore National Laboratory, and six university partners. The prototype TPC met a Level-II milestone for the Weapons Program Campaign 1.

Another great recent success was the installation and commissioning of the Mark-III target. Another great example of teamwork and dedication!

With the intent of continuing communication and keeping the LANSCE community informed, I'm planning to send a periodic e-mail to the entire LANSCE User Community (TA-53 included of course). The first e-mail was sent on October 13 as "LANSCE User Program Headlines, No. 1." Please take a look when you have a chance, feedback is welcome as well.

We will be hosting the 2010 LANSCE Advisory Board Meeting, October 24-26. We have a very interesting agenda with good representation of all of our science programs, from pRad to Lujan Center, including IPF, UCN, and WNR. I hope that in my next "From the Desk" I'll be able to elaborate the outcome of the meeting.

So, since this is my first from LANSCE's DO Desk, please give me some feedback. Also stop by or invite me anytime for a science chat and/or instrument/experiment tour....Gets pretty lonely here.

LANSCE Deputy Division Leader Alex Lacerda

Tovesson... energy range, allowing for unprecedented accuracy in observing neutron-induced fission events. The research is funded by the Department of Energy.

Previous fission detectors only registered quantity and magnitude of events. The Time Projection Chamber will reconstruct a track for each fragment detected, thus allowing for identification of all charged particles emitted from fission and other reactions, as well as the removal of backgrounds that limited the accuracy of previous measurements, and enabling a better understanding of systematic errors.

"I am very excited about this new instrument, not only for measuring fission cross sections, but also for all the possibilities it opens up," Tovesson said. "Nuclear fission is a highly complex process, and there are many unanswered questions related to this nuclear reaction. By studying properties of radiation emitted, such as mass yields of the fission products, one can gain insight in the process and hopefully improve current models of fission."

Tovesson also leads the experimental work for the Spectrometer for Ion Detection Fission in Fission Research (SPIDER). This proposed new instrument at WNR would be used to perform high-precision mass measurements of fission fragments in support of nuclear applications and improvement in theoretical modeling of the fission process.

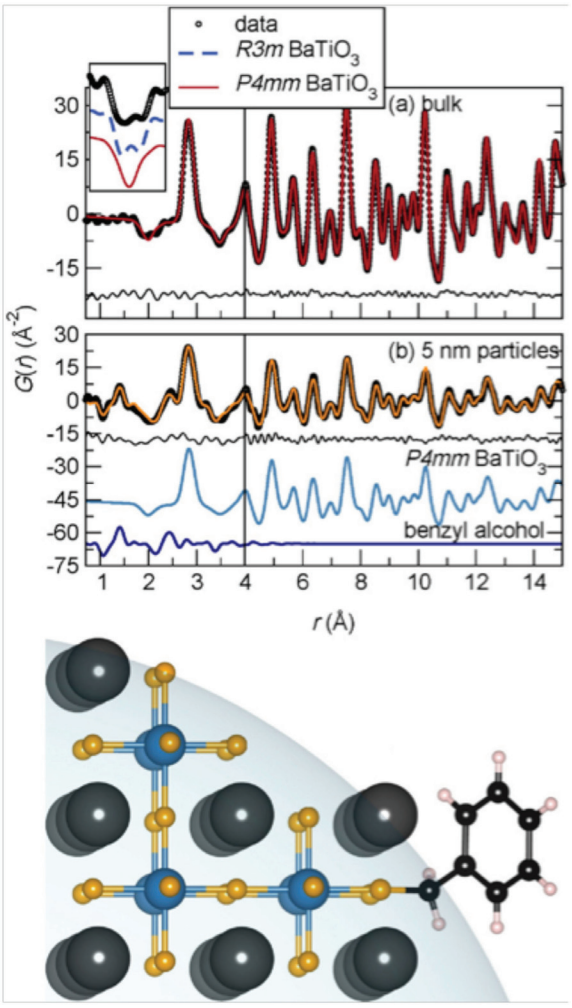
The SPIDER team, which includes scientists from LANSCE, Computational Physics, Nuclear and Radiochemistry, and Nuclear and Particle Physics, Astrophysics, and Cosmology, received Laboratory Research and Development program reserve funding for 2011 for a feasibility study that will demonstrate the impact the project will have on applications related to national security and advanced nuclear reactors.

"Fredrik is a young, talented and enthusiastic scientist," LANSCE-NS Group Leader Stephen Wender said. "He has a general understanding of fission research and has a lot of passion for his research."

Probing local dipoles and ligand structure in $BaTiO_3$ nanoparticles

Katharine Page and Thomas Proffen (Lujan Center, LANSCE-LC) and collaborators Markus Niederberger (ETH Zurich) and Ram Seshadri (University of California, Santa Barbara) have used total scattering neutron pair distribution function analysis to compare the structure of 5-nm particles of the canonical perovskite ferroelectric $BaTiO_3$ to the structure of the bulk material. The results revealed features of titanium-oxygen distances that are not well probed with x-ray scattering.

$BaTiO_3$ is a material of scientific interest because its high dielectric constant and room temperature ferroelectric behavior make it ideal for use in electronic components, such as multilayer capacitors and piezoelectric transducers. Moreover, high dielectric ceramics are currently in great demand because they can make materials lighter and smaller. $BaTiO_3$ has four crystallographic phases, each with a distinct dielectric behavior. Changes in symmetry arise from the displacement of titanium atoms from the center of the oxygen octahedra, causing spontaneous polarization.



Neutron pair distribution function G(r) analysis of (a) bulk and (b) 5 nm $BaTiO_3$. Experimental data are displayed as points and fits and differences with lines. In panel (a) bulk $BaTiO_3$ is well described by the P4mm structure, except for the nearest neighbor Ti−O distance near 2 Å displayed in the inset, which is split in a manner reminiscent of the structure of rhombohedral R3m rather than tetragonal P4mm $BaTiO_3$. The peak is negative because of the negative scattering length of Ti. The nanoparticle G(r) requires contributions from P4mm $BaTiO_3$ as well as benzyl alcohol to fit the experimental data. The schematic image below depicts part of the nanoparticle, near the surface, with a single capping benzyloxy group.

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Probing . . . Ferroelectricity is frequently suppressed in $BaTiO_3$ architectures with one or more diminished dimensions. Because critical size effects will define the extent to which these materials can be incorporated into future generations of electronic devices, the scientists investigated $BaTiO_3$ nanoparticles to determine the degree to which these materials can be downsized and remain functional.

The researchers used the Neutron Powder Diffractometer at the Lujan Neutron Scattering Center for neutron total scattering to study the dipole correlations in a sample of freestanding, capped $BaTiO_3$ nanoparticles. The research addressed structural off-centering, the molecular basis for the existence of switchable dipoles in polar materials, and whether it is turned off when particles become very small. The studies revealed the atomic correlations of the nanoparticle oxide and the capping benzyloxy ligand groups, and allowed careful comparison with the structure of bulk $BaTiO_3$. Even at these small sizes, titanium is locally strongly off-centered. The results revealed that small $BaTiO_3$ particles are more cubic, because of decreased dipole-dipole correlations, while retaining the tetragonal distortion similar to bulk $BaTiO_3$ locally.

The demonstrated probing of both the atomic structure of the oxide core and organic capping components with neutrons heralds a closer examination of other hybrid organic-inorganic systems and the roles that size dependence, defect structure, surface chemistry, and other effects play in determining material properties in numerous functional nanosystems. These effects are of fundamental interest because they will define the extent to which nanomaterials can be incorporated into future generations of electronic devices.

Reference: "Probing Local Dipoles and Ligand Structure in $BaTiO_3$ Nanoparticles," *Chemistry of Materials* **22**, 4386 (2010). The DOE Office of Basic Energy Sciences funds the work.
Technical contact: Katharine Page

LANSCE helps to reveal the first structural details of an HIV-related protein

Jarek Majewski (LANSCE-LC) and collaborators have used neutron scattering to reveal the first structural details of a key protein found in the human immunodeficiency virus (HIV-1). Their work may have important ramifications for the study of the causes and treatment of HIV.

HIV-1 encodes six accessory proteins, including the *Nef* protein. *Nef* is expressed in high concentrations shortly after viral infection, is required for achieving and maintaining high viral loads, and plays a role in AIDS progression. Clinical studies of long-term HIV-infected humans with apparent deletions and/or alterations within the *Nef* gene showed impaired progression to AIDS. Because the Nef protein is an important factor for the progression of AIDS, obtaining details about its function is extremely desirable. Many of the functions of *Nef* appear to be structurally driven or intimately tied to conformation and conformational changes. In addition, cell membrane association plays an important role in many of the functions of *Nef*.

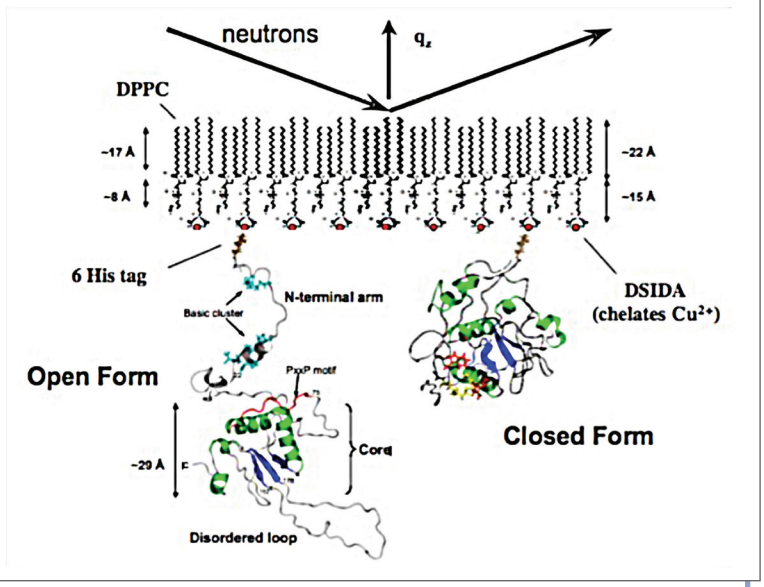

Illustration of the experimental system. The model lipid membrane composed of DPPC {1,2-dipalmitoyl-sn-glycero-3-[phosphocholine]} and charged DSIDA (1,2-distearylglycero-3-triethyleneoxideiminodiacetic acid) molecules is created at the air-liquid interface. Molecules of Nef proteins are injected into the liquid subphase, and their structural conformations (here shown in the "open" and "closed" forms) are studied using neutron reflectometry.

In spite of the wealth of knowledge about what *Nef* does, there is much less information about how it accomplishes its functions. Knowledge of *Nef* structure-function relationships both in solution and in association with lipid membranes is important for understanding and combating the actions of *Nef* in vivo. Such an endeavor requires conformational details about *Nef*. It has been hypothesized that a transition from a "closed" conformational form to an "open" form enables interaction of *Nef* with cellular proteins. However, obtaining structural information about *Nef*, particularly when associated with membranes, is difficult. The full-length *Nef* protein is partially disordered and contains intrinsically flexible regions.

Neutron reflectometry is one of a few methods that can resolve structural details of membrane-associated proteins in physiological conditions. It may be unique in its ability to directly resolve

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Reveal . . . details of the full membrane-bound protein structure. Majewski and collaborators [M. S. Kent and J. K. Murton (Sandia National Laboratories), S. Satija, B. Akgun, H. Nanda, and J. E. Curtis (National Institute of Standards and Technology); C. R. Morgan and J. R. Engen (Northeastern University)] have performed the first in-situ "visualization" of the *Nef* protein structure interacting with model lipid membrane. The scientists found that the *Nef* core domain is located within a few Angstroms of the lipid headgroups of the membrane. This result indicates that the *Nef* protein structure is compact. Analysis involving a simulated ensemble of conformations suggests that the disordered loop extends from the core domain. The researchers conclude that a small portion of *Nef's* N-terminal arm inserts into the membrane.

Reference: "A Study of the Conformation of HIV Nef Bound to Lipid Membranes by Neutron Reflectometry," *Biophysical Journal* in press. The DOE Office of Basic Energy Sciences supported the Los Alamos portion of the research.

Lujan Center researcher recognized at annual Technology Transfer ceremony

LANSCE-LC researcher Michal Mocko was among the recipients of the Programmatic Impact Award at the recent 12th Annual Technology Transfer Recognition and Awards reception.

Mocko was a member of a Laboratory team honored for their efforts in the Stand-Off Radiation Detection System Program. The U.S. Department of Homeland Security's Domestic Nuclear Detection Office has the goal to develop advanced nuclear detectors that can autonomously determine the type and location of radiation sources at much greater distances than current technology. These detectors would help to protect the U.S. The Los Alamos team partnered with major defense contractors to demonstrate the new system in the field.

Steve Girrens presents awards to Larry Schultz, Michal Mocko, David Palmer, Shawn Tornga, and Andrew Hoover.

Team members included Mocko, Mark Wallace (Global Security Programs, GS-PO), Shawn Tornga, Andrew Hoover, David Palmer, and Mark Galassi (Space Science and Applications, ISR-1); and Larry Schultz (Applied Modern Physics, P-21).

The Programmatic Impact Award recognizes individuals or groups who have made advancements to the Laboratory's programmatic mission through their interactions with industry partners.

The awards honor Laboratory scientists and technicians who develop scientific technologies in support of the Laboratory's mission. These technologies also have great potential for commercialization in business and industry. The event recognized contributors to the protection and transfer of technology through patents, copyrights, cooperative development agreements, and licenses. Distinguished Awards were given for accomplishments in patenting, copyright, licensing, programmatic impact, and regional impact during fiscal year 2009.

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Celebrating service

Congratulations to the following LANSCE and AOT Division employees celebrating service anniversaries this month:

Peter Prince, LANSCE-DO	25 years
Eric Olivas, AOT-MDE	15 years
Diana Baker, AOT-MDE	5 years

HeadsUP!

Be sure to enter your T&L on time

The Associate Directorate for Experimental Physical Sciences has recently issued Oracle Time and Labor Guidance for Timekeepers that affects those who do not meet the deadline for time and labor entry. ADEPS is following CFO guidance for OTL timekeepers presented at the All Managers' Meeting September 21, 2010 by Scott Larkin, which states *"For employees who have not submitted a timecard by 9:00 a.m., instruct timekeepers to charge the employee's vacation, or leave without pay if the employee does not have sufficient accrued vacation."* For the specfic actions in this guidance, please see ADEPS 10-011 OTL Guidance for Timekeepers, at int.lanl.gov/orgs/adeps/policy.shtml.

Safe driving includes being familiar with a vehicle before operating it

The number one DOE activity that results in fatalities is something that everyone does each day – Driving! From 1999 through 2009, there were 13 motor vehicle-related deaths out of 26 total DOE fatalities. More recently, from 2008 through 2009, there were 4 DOE motor vehicle-related fatalities.

DOE has many different makes and models of motor vehicles that are driven by employees in the daily performance of work. Evidence exists that drivers may not be sufficiently familiar with the operating controls and other features of a vehicle before they adjust them while driving. Being distracted (searching for unfamiliar vehicle controls) while operating a motor vehicle is the surest way to have an accident. Many long-term university research projects have consistently demonstrated that distracted driving affects reaction times in a manner that is very similar to driving under the influence of drugs or alcohol.

In the October 2010 Office of Health, Safety and Security Just-in-Time Report on this topic, several cases, one a fatality, are described that involved drivers trying to find the parking brake release lever on government vehicles they were operating. The simpliest task can turn deadly in unfamiliar settings.

Coyote Call Trail, Valles Caldera