The Nuclear Process Science Initiative (NPSI) is a Pacific Northwest National Laboratory (PNNL) internally-funded effort to advance nuclear process science capabilities to meet national needs in environmental management, nonproliferation and other areas. The five-year initiative was launched in mid-2015.

***NPSI's vision** is to understand, harness, and exploit interfacial phenomena controlling the behavior of materials in nuclear processing.*

Researchers are working in three "thrust" areas:

***Science Thrust 1**:*
Legacy Waste

***Science Thrust 2**:*
Nuclear Security

***Science Thrust 3**:*
Analytical Capabilities

April 2018

Reid's Notes

NPSI Makes Changes to Science Thrusts to Drive Initiative Outcomes and Strengthen Linkages with the Radiochemical Processing Laboratory (RPL)

By Reid Peterson, Initiative Lead

As initiatives mature, they naturally start to look to the future, and the transition of the projects to client-funded activities. As part of that transition, NPSI recently introduced a new organizational framework for our research that links initiative projects more clearly to mission outcomes.

While some might be tempted to view this as a cosmetic change only, it's more than that. We're confident this new structure will enhance synergy between our projects, strengthen outcomes, and provide our prospective clients with a better understanding of what NPSI is delivering. In addition, the structure allows us to more clearly reflect the foundational role PNNL's RPL plays in this initiative and, likewise, how NPSI's interconnected

NPSI Leadership:

Initiative Lead: Reid Peterson
Deputy Lead: Brienne Seiner
Thrust 1 Lead: Reid Peterson
Thrust 2 Lead: Jon Schwantes
Thrust 3 Lead: Kevin Rosso
Project Coordinator: Barb Beller
Finance: Debbie Lucas
Communications: Tim Ledbetter

Visit the NPSI Website
Contact Us

New Project Gets Under Way

NPSI has recently launched a new project, bringing the total number of active projects to 16.

"Controlled Mineral Growth for Improving Tc-99 and I-129 Retention in Cementitious Waste Forms" is led by **Sarah Saslow**, a scientist in PNNL's Energy and Environment Directorate (EED).

Sarah Saslow

The project will probe solid-liquid interfacial transformations that drive the retention and release of technetium-99 and iodine-129 from mineral phases found in cementitious waste forms.

Understanding these physiochemical properties and reactions will help guide technical cementitious waste form contributions help enhance the RPL's status as a premier national research facility.

Under the new structure, NPSI's three research "thrust areas" are now:

- **Legacy Waste**
- **Nuclear Security**
- **Analytical Capabilities**.

Each of our current projects is housed in one of the thrust areas. This isn't so different from our previous structure--we had three thrust areas then, too, but they were described as specific science disciplines. Now, our thrusts and associated projects not only "map" more clearly to RPL capabilities, but are more descriptive of the outcomes we're seeking for our clients and the nation--contributions to environmental cleanup, national security and associated analytical methods and tools.

We're still refining the words we use to describe each thrust area, but for a general understanding of how the thrusts and projects fit together, please take a look at the NPSI overview flier on our website.

Reid

NPSI Team to Author Book on Engineering Separations

NPSI Lead **Reid Peterson** and several of the initiative's researchers have started work on a new book tentatively titled, "Engineering Separations Unit Operations for Nuclear Processing." Earlier this year, PNNL reached agreement with CRC Press-Taylor & Francis Group, which had approached Peterson about developing the book.

"The topical area aligns with work we're doing in NPSI, and we will augment the writing done here with content from non-PNNL researchers we've enlisted to participate. The book will cover a discipline in nuclear process science that is key to waste processing, but hasn't been widely addressed in academia or industry," Peterson says.

The authors will deliver about 400 manuscript pages and 100 figures next spring, after which the publisher will begin

developments that will directly benefit the disposal needs of the Hanford Site's low activity waste and secondary waste streams.

Paper Offers Insights into Hanford Tank Waste

A NPSI-funded paper provides a view into the millions of gallons of radioactive waste stored in the Hanford Site's underground tanks and offers new understanding of tank waste properties.

The paper, "Review of the Scientific Understanding of Radioactive Waste at the U.S. DOE Hanford Site," was published in January in *Environmental Science and Technology*.

The authors include **Reid Peterson**, **Edgar Buck**, **Jaehun Chun**, **Richard Daniel**, **Eugene Ilton** and **Gregg Lumetta** of PNNL; **Daniel Herting** of Washington River Protection Solutions; and **Sue Clark**, who serves in a joint PNNL-Washington State University appointment and previously led NPSI.

Read more about the paper on the NPSI website.

the editing process. In addition to Peterson, NPSI's **Amanda Casella**, **Philip Schonewill** and **Cal Delegard** are handling author duties.

NPSI Advances Capabilities. . .

Years of Effort Culminate in Unique Plutonium Experiment

A groundbreaking experiment at PNNL that employed novel methods to safely create and analyze plutonium samples could prove influential in future studies of the radioactive material.

Dallas Reilly

"The experiment has thus far provided interesting preliminary data," says researcher **Dallas Reilly**, "but the methods we used to conduct the work will be of high interest to national laboratory and university communities, and could help advance research in legacy waste, national security, and even nuclear fuels." The experiment was funded through two PNNL Laboratory Directed Research and Development (LDRD) program efforts: NPSI and an Open Call project Reilly led.

The experiment started with a nine-gram ingot of plutonium metal produced in the Radiochemical Processing Laboratory. In December 2017, the material was placed in a focused ion beam instrument, or "FIB," at RPL. The instrument was used to remove smaller samples from the metal, and then shape those samples into tiny "needles."

Sweet to Present at X-ray Conference

Luke Sweet, who leads the NPSI project, "*Characterization of Radiation Induced Materials Defects Across Scales*," has been invited to co-present a workshop at a premier international meeting this summer.

The workshop will focus on X-ray diffraction line profile analysis, and will be held as part of the Denver X-ray Conference set for August 6-10 in Westminster, Colorado. The conference is sponsored by the International Centre for Diffraction Data.

The invitation is a recognition of Sweet's expertise in diffraction analysis. The half-day educational and training workshop will be led by Matteo Leoni from the University of Trento. In addition to Sweet, two representatives from the National Institute of Standards and Technology will provide presentations.

Separate from the workshop, Sweet and colleague **Jordan Corbey** are in the process of submitting abstracts to the conference for a talk and poster specific to the work they're doing on microstructure properties quantification in Sweet's NPSI project. The project is part of the initiative's Analytical Capabilities thrust.

Next, Dallas explains, the needles were "free-released" (a process that enables movement of minuscule quantities of radioactive material without radiological controls) and carefully transported to the Environmental Molecular Sciences Laboratory (EMSL), a DOE Office of Science User Facility located at PNNL. At EMSL, the needles were placed in an Atom Probe Tomography (APT) instrument, which sheds atoms, one small layer at a time, from each needle. The atoms were detected and then factored into mathematical formulas to help create a "reconstruction"--essentially a 3-D graphical atom-by-atom representation of each needle.

Although the reconstruction provided some interesting insights about the material, the more noteworthy aspect of the experiment was the sample creation and analysis process. The ability to move a plutonium sample from the RPL, a Hazard Category II Non-Reactor Nuclear Facility, to a non-radiological facility like EMSL--and then safely use instrumentation not available at RPL--is a major step forward in more fully tapping research capabilities at PNNL.

The planning for this type of experiment started a number of years ago and over time has involved multiple PNNL research directorates, as well as numerous health and safety experts. Dallas was part of a team that approximately two years ago put forward a free release workflow document to enable easier, and safe, movement of tiny samples outside of radiological controls if certain thresholds, including Nuclear Regulatory Commission surface contamination limits, are met. The free release workflow, coupled with a diligent staff effort to ensure necessary health and safety requirements were in place, facilitated the APT experiment.

"For the experiment itself, several of us worked long hours for three days, but we successfully completed the task, and did so safely," Dallas explains. "There are risks in a project like this, but we managed the risks in an intelligent, thoughtful way, aligned with stringent safety standards."

Dallas believes the experimental results could contribute to two journal papers, and he's also hoping to share similar information at the Plutonium Futures conference later this year. He and colleagues next plan to use the same experimentation process in another LDRD project to study plutonium particles from the Hanford Site, which will reveal information about particle composition. Such new knowledge could help inform waste cleanup strategies, and

Staff Recognition

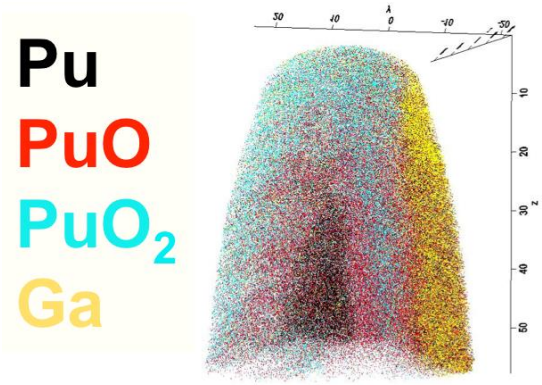
Analytical Capabilities Thrust Area Lead **Kevin Rosso** has been appointed to a National Academies of Sciences, Engineering and Medicine (NASEM) committee. The committee will develop the agenda for basic research in separations science. Rosso was asked to join based on his expertise in molecular interfaces. More info. . .

Also, former NPSI Lead **Sue Clark** has been appointed to a NASEM Committee to evaluate the U.S. Department of Energy's cleanup technology development efforts. Clark currently serves as the EED Chief Science and Technology Officer at PNNL. More info. . .

Philip Schonewill, who works on the Legacy Waste Thrust Area's filtration project, was a finalist for EED's Project Manager of the Year Award. He was cited for his management of the Washington River Protection Solutions Low Activity Waste Pretreatment System Integrated Testing Project, and was honored during EED's annual "Of-the-Year"

also help demonstrate PNNL's advanced research capabilities to the broader scientific community.

The experiment team included Dallas, who works in PNNL's National Security Directorate (NSD); **Daniel Perea**, Earth and Biological Sciences Directorate (EBSD); **Timothy Lach**, Energy and Environment Directorate (EED); **Amanda Casella** (EED); **Marie McCoy** (NSD); **Karl Pitts** (NSD); and **Jon Schwantes** (NSD). The experiment was funded through the NPSI project, *Monitoring Diffusion of Actinide Daughters and Granddaughters in Metals for Chronometer Applications*, and the LDRD Open Call project, *Hot Particle Analysis Aided by a State-of-the-Art Focused Ion Beam.* Reilly leads both projects.



The experiment produced a 3-D graphical atom-by-atom representation of each needle--in this case showing plutonium, plutonium oxide, plutonium dioxide and gallium components.

Seiner Takes on Role of Deputy Initiative Lead

Brienne Seiner has joined NPSI as the deputy lead, succeeding **Matt Douglas**, who had served in the position since NPSI's early days.

Brienne Seiner

"We thank Matt for his outstanding service to NPSI, and look forward to working with Brienne and benefitting

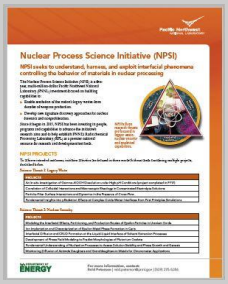
ceremony in December.

NPSI Deputy Lead **Brienne Seiner** received the Core Values Award during the PNNL NSD's "Of the Year" award ceremony in December.

Visit the NPSI Website for the Latest Updates

The website is regularly updated and offers the latest information on NPSI and its research.

One recent addition to the site is an overview flier that highlights NPSI's vision, objectives, research thrust areas and projects.



from her knowledge and leadership," says NPSI Lead Reid Peterson.

Matt Douglas

Seiner joined PNNL in 2010 and currently is a team lead within the Chemistry of Nuclear Materials group in NSD.

She is a trained radiochemist with experience in inorganic complexation, organic synthesis, chemical separations, and isotope production. At PNNL her focus has been in areas of nuclear nonproliferation detection and analysis in multiple sponsor spaces.

More information about Dr. Seiner is available on the Staff page of the NPSI website.

NPSI Publications

September 2017 - April 2018

Journal Articles:

Pednekar, S., J. Chun, J.F. Morris. 2018. "**Bidisperse and Polydisperse Suspension Rheology at Large Solid Fraction**," *Journal of Rheology*, 62(2): 513-526. DOI: 10.1122/1.5011353. February 2018.

Peterson, R.D., E. Buck, J. Chun, R. Daniel, D. Herting, E. Ilton, G. Lumetta, and S. Clark. 2017. "**Review of the Scientific Understanding of Radioactive Waste at the U.S. DOE Hanford Site**," *Environmental Science & Technology*, 52(2):381-396. DOI: 10.1021/acs.est.7b04077. December 2017.

Wu Z, J. Chun, S. Chatterjee, and D. Li. 2017. "**Fabrication of Oriented Crystals as Force Measurement Tips via Focused Ion Beam and Microlithography Methods**," *Surface and Interface Analysis*. DOI: 10.1002/sia.6346. November 2017.

Jiang W, M.A. Conroy, K. Kruska, N.R. Overman, T.C. Droubay, J. Gigax, L. Shao, and R. Devanathan. 2017. "**Nanoparticle Precipitation in Irradiated and Annealed**

Ceria Doped with Metals for Emulation of Spent Fuels,"
Journal of Physical Chemistry C., 121(40): 22465-22477.
DOI: 10.1021/acs.jpcc.7b06188. September 2017.

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