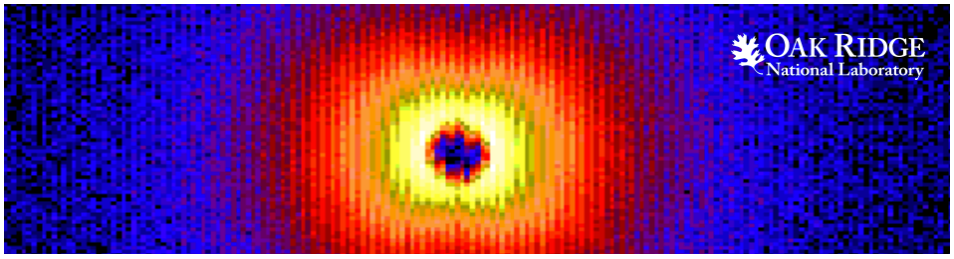
Neutron Sciences in Support of Nuclear Power 2019

Thursday 16 May 2019 - Friday 17 May 2019



Book of Abstracts

Fundamental Molten Salt Research and the Importance of Neutron Studies of Salt Structure

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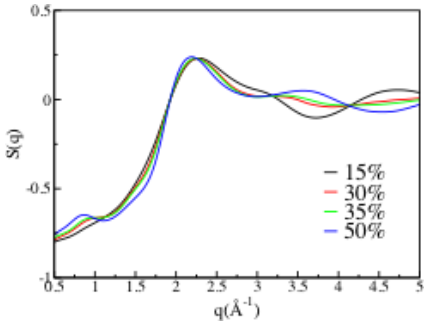
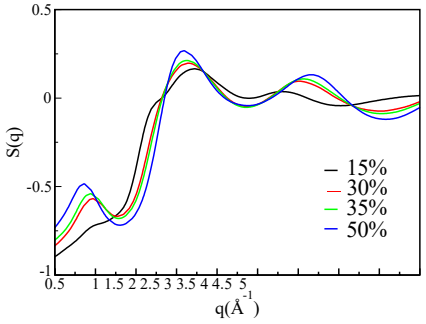
Molten Salt Reactors (MSRs) are a potential game-changing technology that could provide cost-competitive, safeer, and more sustainable commercial nuclear power, and the possibility of a once-through uranium fuel cycle. Molten salts are intrinsically-structured liquids, subject to complex physical and chemical processes. The development of new MSR concepts requires solid understanding of, and predictive models for, the physics and chemistry of molten salts and their behavior with solutes, including actinides, and in contact with nanomaterials and reactor materials. The EFRC for Molten Salts in Extreme Environments (MSEE) seeks fundamental and predictive understanding of molten salt bulk and interfacial chemistry that will establish robust principles to guide the technologies needed to deploy MSRs. The overarching themes of MSEE are (i) Molten Salt Properties and Reactivity, which aims to understand the thermal, radiolytic, redox, and solubility behavior of high-temperature molten salts under reactor conditions, including dissolved actinides and fission products; and (ii) Interfacial and Corrosion Processes in Molten Salt Environments, which aims to understand interfacial and corrosion processes between molten salts and reactor materials, including the effects of radiation and high temperature. A key feature ofMSEE is the close collaboration between theoretical modeling and radiolytic, synchrotron- and neutron-based techniques to build an atomic-level view of molten salt dynamics, structure and chemical reactivity.

We apply theory and molecular dynamics (MD) simulation methods at the electronic and classical levels to provide novel atomistic insights into the structure and dynamics of molten salts. These insights permit us to interpret and derive more information from experimental measurements of structure by high-energy X-ray and neutron scattering techniques at high temperatures. We focus on a series of molten chloride salts with monovalent, divalent, and trivalent cations, and their mixtures, and we model structural, thermodynamic, and transport properties as functions of temperature. We are breaking new ground in molten salt MD simulations, which requires thorough and rigorous comparison between our scattering experiments and our *ab initio* and classical polarizable and nonpolarizable force field molecular dynamics results. This enables us to assess the quality of our parameterizations, and lays a strong foundation for modeling more complex mixtures including fuel salts, corrosion, and fission products. In this talk, we will discuss our advances so far in understanding properties of molten salts such as structure factors, coordination structure, and physical properties, and the importance of neutron scattering in the interpretation of molten salt structure via the partitioning of structure factors enabled by the contrast provided by scattering factors and isotopic substitution.

This work was supported as part of the Molten Salts in Extreme Environments Energy Frontier Research Center, funded by the U.S. Department of Energy Office of Science.



Simulated **X-ray** scattering $S(q)$ as a function of $MgCl_2$ concentration in $MgCl_2$-KCl mixtures.



Simulated **neutron** scattering $S(q)$ as a function of $MgCl_2$ concentration in $MgCl_2$-KCl mixtures.

The Fertile Yet Untilled Ground of Neutron Scattering Applied to Hydrogen in Zr-based LWR Alloys

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Department of Nuclear Engineering

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Neutron scattering techniques are ideally suited to study hydrogen in metals such as the Zr-based alloys used for LWR fuel cladding. However, the application of neutron scattering based techniques is under-utilized in this regard. The talk will present a few introductory concepts related to hydrogen in Zr-based alloys and the utility of neutron scattering. The example of nCT and nR to characterize hydride lenses or blisters in Zircaloy 2 will be presented.

Unraveling the Spectroscopic Signatures of Nuclear Waste: What's Next with Neutrons?

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Abstract

The Hanford site in Washington State, which produced plutonium for the US weapons program, is the most contaminated nuclear site in the nation and is its largest environmental clean-up activity. During weapons production, 56 million gallons of liquid radioactive/chemical waste (sludge, salt cake, and supernate), with 170 million Curies of radioactivity and 240,000 tons of complex chemicals, was generated. This liquid waste is the primary environmental contamination risk, currently intended to be processed into a glass form for stabilization and to allow its radioactivity to safely dissipate over hundreds to thousands of years. Uncertainty associated with nuclear waste processing and disposal can be mitigated by: (i) characterizing waste chemistry; and (ii) understanding contaminant reactions both in the waste form and with environment.

A key issue of Hanford tank waste processing and disposal is that, although radionuclides such as technetium are the risk drivers, it is the 'benign' dominant elements such as aluminum (Al) that dictate the processing limits and uncertainties, given that tank waste is removed on a volume basis. Thus, safe, cost-effective, and efficient waste processing depends on a fundamental understanding of aluminum chemistry in these complex high ionic strength, highly alkaline solutions.

Research by the Interfacial Dynamics in Radioactive Environments and Materials (IDREAM) Energy Frontier Research Center (EFRC) has focused on unravelling Al^{3+} ion coordination, solvation, pairing with other ions, and cluster formation in these complex chemical environments. The goal of this research is to understand mechanisms of aluminum speciation changes that underpin nucleation and precipitation, by developing a definitive guide to oligomeric Al signatures from multiple spectroscopic techniques. A combined experimental and theoretical interrogation will be presented to predict dynamic solute and solvent behavior in these concentrated systems, where ions must share dilute water molecules with each other.

Biographical Sketch

Carolyn Pearce joined PNNL in 2016 and works on the characterization of solutions and minerals relevant to radioactive waste storage and processing in order to determine reaction mechanisms and kinetics that affect radionuclide stability in waste forms and subsurface environments. Dr. Pearce leads research programs for US DOE Office of Science, Office of River Protection, Environmental Management and has an international perspective on the science of nuclear waste processing and management. Dr. Pearce obtained her B.Sc. and PhD from the University of Leeds, UK, and is a visiting academic in the Department of Crop and Soil Sciences, Washington State University, and the School of Earth and Environmental Sciences at the University of Manchester, UK.

The Application of Advanced Microstructural Characterization Techniques for Investigating the Performance of Neutron-irradiated U-Mo Alloys

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ABSTRACT

The Material Management and Minimization (M3) Program is developing low enriched uranium fuels for application in research and test reactors. One plate-type fuel is a U-Mo monolithic fuel, and the second is a U-Mo dispersion fuel. To successfully qualify these fuel types, it is important to have good understanding of their fuel performance under different irradiation conditions. In the last few years, a variety of advanced microstructural characerization tools have become available at the Idaho National Laboratory for characterizing different nuclear fuel types that have been irradiated to high fission density. This presentation will highlight how these tools have been used by the M3 program to provide new information about the microstructual evolution of U-Mo alloys during irradiation. Some of the techniques that have been employed include high-resolution transmission electron microscopy, atom probe tomography, electron energy loss spectroscopy, and electron backscattered diffraction. Information like that generated from this work is key for improving computer modeling of the fuel performance under irradiation. The results generated to data have been used to improve understanding of phenomena like recrystallization/polygonization, grain growth, radiation stability, and swelling of irradiated U-Mo fuel and other fuel plate materials.

Using Good Neutrons (SANS) to Fight Bad Neutrons (Radiation Damage)

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Abstract

The continued safe operation of nuclear reactors and their potential for lifetime extension depends on ensuring reactor pressure vessel (RPV) integrity, which embrittles as a result of neutron exposure, and the radiation damage caused by bad neutrons. The microscopic cause of this RPV embrittlement is now well established to be the formation of a high number density of nanometer-sized copper rich precipitates and sub-nanometer defect-solute clusters during neutron exposure. The use of good neutrons through the use of small angle neutron scattering has been instrumental in confirming the role of copper rich precipitates and to resolving technical disagreements about the composition of these nanometer-sized precipitates. In this presentation, we will review the use of SANS, in combination with other techniques such as Atom Probe Tomography, positron annihilation spectroscopy and a novel, temperature-dependent SANS measurement to quantify the precipitate size, number density and composition of these embrittling precipitates in Fe-based model alloys, as well as actual RPV surveillance specimens. The various characterization methods show relatively good overall consistency with regard to the Cu-rich precipitate number densities, volume fractions and sizes. However, the nominally high concentrations of Fe in the precipitates are shown to be an atom probe artifact.

SANS and Neutron Diffraction Studies of Fusion Reactor Materials and Components

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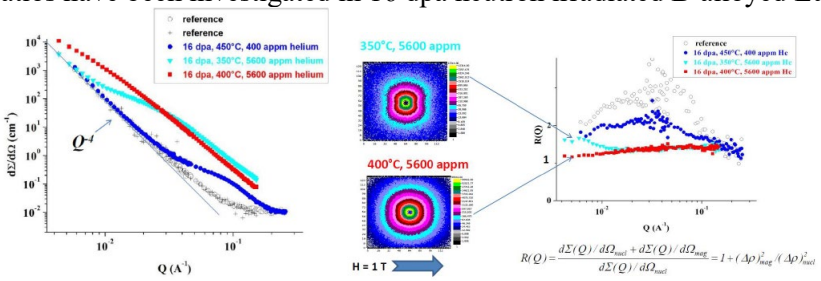
The design of future *tokamak* based fusion reactors requires to develop innovative structural materials and components capable to withstand the unprecedented service conditions expected for such machines. Namely, helium/dpa (displacement per atom) ratios one order of magnitude larger than in fusion reactors will be produced in the structural materials by the 14 MeV neutron flux. Furthermore, high temperature materials are needed to construct plasma-facing components, such as the *divertor*, capable to contain as much as possible disruptive phenomena, originated by plasma instabilities.

This contribution will present original experimental results, obtained by Small-Angle Neutron Scattering (SANS) and neutron diffraction, in the frame of the EUROfusion research programme. SANS is providing useful information to quantitatively characterize the micro-structural radiation damage in ferritic/martensitic steels (Eurofer97) developed for the *first-wall* and other structural components. The effects of high He/dpa ratios have been investigated in 16 dpa neutron irradiated B-alloyed Eurofer97 steel (1).



Neutron diffraction provides bulk values of the stress field in brazed W-Cu *divertor* components, allowing a comparison with the theoretical predictions obtained by numerical methods (2).

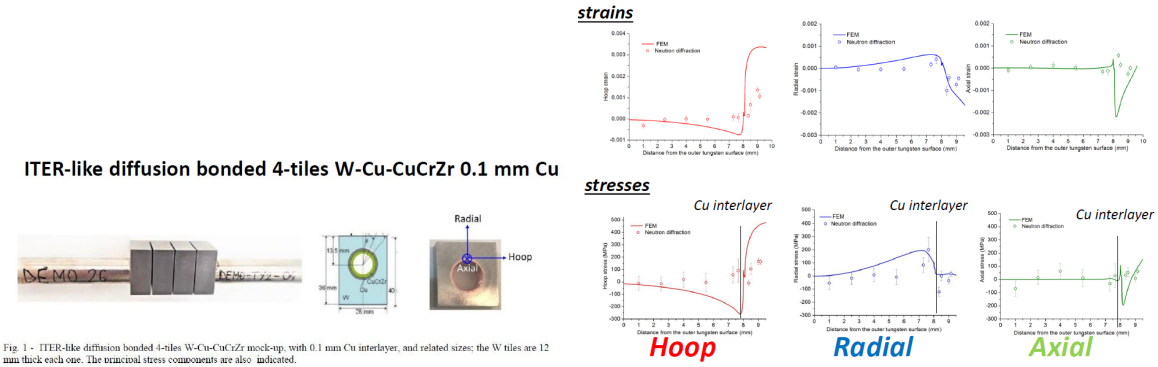


Fig. 1 - ITER-like diffusion bonded 4-tiles W-Cu-CuCrZr mock-up, with 0.1 mm Cu interlayer, and related sizes; the W tiles are 12 mm thick each one. The principal stress components are also indicated.

1. R. Coppola, M. Klimenkov, A. Möslang, R. Lindau, M. Rieth, M. Valli, *Micro-structural effects of irradiation temperature and helium content in neutron irradiated B-alloyed Eurofer97-1*, Nucl. Mat. En. 17 (2018) 40-47

2. R. Coppola, F. Crescenzi, W. Gan, M. Hofmann, M. Li, E. Visca, J.-H. You, *Neutron diffraction measurement of residual stresses in an ITER-like tungsten-monoblock type plasma-facing component*, Fus. Eng. & Des. (2019) in print

Thermal Neutron Scattering: Defining the Physics of Power Reactors

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Abstract

Thermal neutron scattering has long been a technique for probing matter. From a nuclear power perspective, thermal scattering fundamentally defines the operational and safety behavior of the current fleet of nuclear power reactors (national and international). Moreover, some of the most promising concepts of advanced reactors that are expected to be deployed in the next 20 years, such as high temperature and molten salt reactors, are also driven by thermal fission. In all these reactors, energetic neutrons born in fission moderate by elastic down scattering until reaching the thermal region. At this stage, the neutrons initiate a two-way interaction process (up and down scattering) with the core environment, especially the moderator, that samples its available energy and momentum states. This "thermalization" process establishes a quasi-equilibrium thermal neutron spectrum in the core. It is quantified using the moderator's dynamic structure factor, which is also known as the thermal scattering law (TSL), i.e., $S(\alpha,\beta)$, where α and β represent dimensionless momentum and energy exchange variables, respectively. Traditionally, $S(\alpha,\beta)$ was estimated using simplifications motivated mainly by computational feasibility. However, modern approaches have emerged that implement atomistic simulations in TSL analysis. To date, much work was performed to develop such approaches and to define experiments for the validation of the generated data. This includes neutron scattering, transmission, and pulsed slowing-down-time experiments that can be used for data validation in the thermal range.

Biographical Sketch

Ayman Hawari is Distinguished Professor of Nuclear Engineering and Director of the Nuclear Reactor Program at North Carolina State University (NCSU). He obtained a BS from the University of Missouri-Rolla and MSE and PhD from the University of Michigan-Ann Arbor, all in Nuclear Engineering. His technical interests include fundamental research on neutron thermalization in matter, radiation measurements for data validation and materials nondestructive examination, and the development and utilization of intense radiation sources (e.g., research reactors and accelerators). He chairs OECD/NEA's subgroup 42 on "Thermal Neutron Scattering Law Data", is a member of NNSA's Nuclear Data Advisory Group (NDAG), and a member of the steering committee for the International Group on Research Reactors (IGORR). His NCSU group is a primary contributor of thermal scattering law data to the recent Evaluated Nuclear Data File (ENDF/B-VIII.0) release. He is a recipient of the NCSU Alcoa Foundation Engineering Research Achievement award and is a Fellow of the American Nuclear Society.

Connecting Processing, Structure, Properties, and Performance in Metallic Nuclear Fuels by Using Neutrons as a Diagnostic tool and to create damage

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Purdue University

Abstract

Metallic nuclear fuels have been historically used in a wide variety of reactor types. More recently, these fuels are under development for high performance research and test reactors, as well as under consideration for use in advanced reactors such as the Versatile Test Reactor, a fast reactor. In order to develop fuel for these reactors, understanding how the fabrication steps impact the microstructure and properties can be important since these characteristics can dictate in-reactor performance. The use of neutron diffraction as an in situ and ex situ tool to characterize the microstructure and mechanical properties of metallic nuclear fuels will be discussed. Also, a recent irradiation vehicle design to capture low fluence neutron damage behavior to enable early insight into fuel performance will be discussed.

Characterization of Solvating Extractants in f-Element Separations

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Supramolecular assembly has been integral to the management of used nuclear fuel since the initial, ether-based solvent extraction process used to purify uranium and attempted during the Manhattan project. Solvating extractants, which rely on supramolecular assembly, are an ideal partner for purifying the *f*-elements away from the rest of the periodic table. The general mechanism for metal recovery by a solvating reagent includes the interaction of a charge neutral, strong dipole amphiphile and charge balancing counter ions with a metal center to solubilize this metal center into the organic phase. This general mechanism is well depicted by a coordination chemistry model, where the metal sits in the center of the coordination complex and the amphiphile and counter-ions populate the metal coordination sphere, however this mechanism probably underestimates the importance of hydrogen bonding and other ion-dipole interactions that control intermediate (second and third coordination shell) and long (bulk material) range interactions. These interactions can control other important phenomena, such as third phase formation, and the combination of X-ray scattering techniques and molecular dynamics simulation is proving to be a powerful partnership in providing molecular level resolution with experimentally determined measurables. This presentation will be an overview of recent findings from this research group, as well as a review of the broader literature pertaining to solvating extractants and extractant aggregation, to highlight the opportunities for using beamline techniques to examine extraction mechanisms most relevant to *f*-element science.