Monday Afternoon, October 21, 2019

Actinides and Rare Earths Focus Topic Room A215 - Session AC-MoA

Early Career Scientists

Moderators: Art Nelson, Lawrence Livermore National Laboratory, David Shuh, Lawrence Berkeley National Laboratory, Evgeniya Tereshina-Chitrova, Charles University, Prague, Czech Republic

1:40pm AC-MoA-1 Advanced Characterization of Nuclear Fuels, Lingfeng He, T Yao, Idaho National Laboratory; V Chauhan, The Ohio State University; A Sen, Purdue University; Z Hua, M Bachhav, Idaho National Laboratory; M Khafizov, The Ohio State University; J Wharry, Purdue University; M Mann, Air Force Research Laboratory; T Wiss, European Commission, Joint Research Centre (JRC); J Gan, D Hurley, Idaho National Laboratory INVITED

Oxide nuclear fuels have been widely used in light water reactors. The thermal conductivity of nuclear fuels is closely related to energy conversion efficiency as well as reactor safety. Understanding the mechanisms that cause the degradation in thermal conductivity in a high radiation environment is important for the design and development of new highburnup fuels. For oxide nuclear fuels, phonon scattering by point defects, extended defects such as dislocation loops and bubbles, and grain boundaries plays a significant role in limiting the thermal transport properties. In this work, detailed microstructural characterization of pristine and ion irradiated ThO2 and UO2 has been performed by using electron backscatter diffraction (EBSD), atomic-resolution scanning transmission electron microscope (S/TEM), atom probe tomography (APT) and time-domain Brillouin scattering (TDBS) techniques. The thermal conductivity before and after irradiation has been determined using laserbased modulated thermoreflectance (MTR) technique. This work is partially supported by the Center for Thermal Energy Transport under Irradiation, an Energy Frontier Research Center funded by the U.S. Department of Energy Office of Sciences.

2:20pm AC-MoA-3 The Influence of Relative Humidity on the Oxidation of δ -Pu, Scott Donald, J Stanford, A Nelson, B McLean, Lawrence Livermore National Laboratory INVITED

The evolution of delta stabilized plutonium aged under a controlled environment composed of laboratory air and a range of relative humidities up to 95% was studied using Auger electron spectroscopy (AES). Linear-least squares analysis was performed on AES spectra acquired during Ar⁺ sputter depth profiles to gain insight on the thickness and any variation in the chemical speciation of the oxide. Sputter rates were calibrated from depth profiles obtained from an oxide of a known thickness from FIB/SEM measurements. At all relative humidities, the initial oxide layer was found to grow logarithmically, indicative of a diffusion-controlled process. The rate of oxide growth was also found to be independent of oxygen partial pressure (for $pO_2 > 31.5$ Torr) for all conditions studied.

The work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

3:00pm AC-MoA-5 Magnetization and Transport Properties of Delta Phase Uranium, Xiaxin Ding, N Poudel, T Yao, J Harp, K Gofryk, Idaho National Laboratory

At room temperature, uranium metal is in its alpha form, the most common structural form of the element. It consists of corrugated sheets of atoms in an asymmetrical orthorhombic structure. However, the room temperature stabilized delta phase can be formed by alloying uranium with zirconium, which is known to have hexagonal crystal structure. It is important to know the physical properties of U-Zr alloys due to their technological importance. In this talk, we will present the first-time results of magnetization, transport and thermodynamic measurements of delta phase uranium at low temperatures and under high magnetic fields. The results obtained help us to understand the 5*f* ground state properties in different phases of U. We will discuss implications of these results.

3:20pm AC-MoA-6 Using Fused Filament Fabrication to Develop Customized Materials which Attenuate Ionizing Radiation, Zachary Brounstein, E Murphy, J Dumont, S Talley, K Lee, A Labouriau, Los Alamos National Laboratory

lonizing radiation is of serious consideration in the nuclear industry because protecting workers and instrumentation is of utmost concern when operating equipment that emits potentially hazardous radiation.

Currently, commercial products are readily used as protective barriers, but there are circumstances when these are less than ideal at providing optimal shielding against neutrons and gamma rays^{[1],[2]}. As innovations to nuclear energy technologies continue to progress, developing new materials for radiation shielding grows in importance and need.

In the present work, we used an additive manufacturing (AM) technique known as Fused Filament Fabrication (FFF) to create novel 3D printed materials for radiation shielding. FFF is a layered AM process whereby thermoplastic filaments are heated up to their melting point and extruded into cross-sections of the end product^{[3],[4]}. Because FFF has the capability to create prototypes and end-use parts with fine resolution details and excellent strength-to-weight ratios, the technology is used throughout aerospace, automotive, and medical industries.

Difficulties in creating filaments for FFF arise from fabricating a homogeneous wire that has uniform thickness and a smooth surface. If a filament does not have these initial properties, then either the FFF process will not work or the end product will not be as desired. Creating a homogeneous wire proves more difficult when different base and filler materials are used in the fabrication process, however, this can be solved if the different materials are combined in a liquid solution. Creating a wire of uniform thickness relies heavily on the extrusion process, whereby the temperature and extrusion speed are controlled.

In this study, we have prepared homogeneous filaments with varying processing conditions such as the contribution of additives and the control of extrusion temperature and speed. Thus, we used FFF to create novel filaments to print sheets of customized materials for attenuating ionizing radiation. Irradiating the printed samples was performed at the Los Alamos Neutron Science Center and the Gamma Irradiation Facility by bombarding the customized materials with neutrons and gamma rays, respectively.

References

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3. Guo, N. and M.C. Leu, Frontiers of Mechanical Engineering, 2013. 8(3): p. 215-243.

4. Srivatsan, T.S. et al, Additive Manufacturing: Innovations, Advances, and Applications. CRC Press. 2016. p. 1-48.

4:00pm AC-MoA-8 Thermodynamic and Thermal Transport Properties of Thorium Dioxide single crystals, *Narayan Poudel*, *X Ding*, Idaho National Laboratory; *J Mann*, Air Force Research Laboratory; *K Gofryk*, Idaho National Laboratory

Thorium dioxide (ThO₂) crystalizes into CaF₂-type (fluorite) cubic structure, similar to other members of AnO₂ (An = Th-Am) family. Thorium dioxide forms stoichiometrically and is a wide-gap transparent insulator (Eg~5-6 eV). This material is used as nuclear fuel in certain types of nuclear reactors (CANDU) that might have more advantages than conventional UO₂ based nuclear reactors. It is because of its higher thermal conductivity, higher corrosion resistance, and higher melting point. Despite its importance in nuclear technology, the thermodynamic and thermal transport properties of ThO₂ single crystals have not been studied extensively, especially at low temperatures where many different scattering mechanisms such as boundary, defects, and/or phonon-phonon dominate the heat transport. In this talk, we will present our recent measurements of the heat capacity and thermal conductivity of ThO₂ single crystals, obtained from room temperature down to 2 K. Large and good quality single crystals of ThO₂ have been synthesized by hydrothermal method for this study. We will also compare the result obtained on ThO₂ to UO₂, especially in the context of impact of 5f-electrons on thermodynamic and transport behavior in these materials.

4:20pm AC-MoA-9 Magnetic Nanoparticles for Biomedical Applications, *Iliana Medina-Ramirez*, A Diaz de Leon Olmos, Universidad Autonoma de Aguascalientes, Mexico; J Zapien, City University of Hong Kong

Magnetic nanostructured materials (MNMs) are attractive candidates for biomedical applications because of the highly desirable advantages of magnetic-guided targeting. Furthermore, MNMs can be produced by simple fabrication processes that enable flexibility to modulate their properties and desired bio-activity.

The simultaneous optimization of the bio-activity of interest while simultaneously preventing, or at least minimizing, deleterious side effects is of the outmost importance for critical applications such as the development of magnetic hyperthermia cancer treatment. However, this

Monday Afternoon, October 21, 2019

requires more complex multi-criteria optimization studies. We use Fe₃O₄ and CoFe₂O₄ MNMs prepared by microwave solvothermal method and a citrate surface modification, to modulate their toxicity and stability, as model systems to develop protocols for optimization of therapeutic MNMs. The interaction of surface-modified MNMs with HepG2 cells is evaluated by colorimetric, optical microscopy and Atomic Force Microscopy (AFM) studies for dose. We show that AFM presents important advantages over conventional techniques including information on the potential internalization of MNMs by the cells as function of surface modification. The optimized MNMs in this study present morphological, colloidal, biocompatibility and magnetic properties that make them promising candidates for the development of efficient therapeutic agents for hyperthermia cancer treatment applications.

Author Index

Bold page numbers indicate presenter

— B — Bachhav, M: AC-MoA-1, 1 Brounstein, Z: AC-MoA-6, 1 -C-Chauhan, V: AC-MoA-1, 1 — D — Diaz de Leon Olmos, A: AC-MoA-9, 1 Ding, X: AC-MoA-5, **1**; AC-MoA-8, 1 Donald, S: AC-MoA-3, 1 Dumont, J: AC-MoA-6, 1 -G-Gan, J: AC-MoA-1, 1 Gofryk, K: AC-MoA-5, 1; AC-MoA-8, 1 -H-Harp, J: AC-MoA-5, 1 He, L: AC-MoA-1, **1**

Hua, Z: AC-MoA-1, 1 Hurley, D: AC-MoA-1, 1 - K -Khafizov, M: AC-MoA-1, 1 - L -Labouriau, A: AC-MoA-6, 1 Lee, K: AC-MoA-6, 1 - M -Mann, J: AC-MoA-8, 1 Mann, M: AC-MoA-1, 1 McLean, B: AC-MoA-3, 1 Medina-Ramirez, I: AC-MoA-9, 1 Murphy, E: AC-MoA-6, 1 - N -Nelson, A: AC-MoA-3, 1

- P --Poudel, N: AC-MoA-5, 1; AC-MoA-8, 1 - S --Sen, A: AC-MoA-1, 1 Stanford, J: AC-MoA-3, 1 - T --Talley, S: AC-MoA-6, 1 - W --Wharry, J: AC-MoA-6, 1 Wiss, T: AC-MoA-1, 1 Wiss, T: AC-MoA-1, 1 - Y --Yao, T: AC-MoA-1, 1; AC-MoA-5, 1 - Z --Zapien, J: AC-MoA-9, 1