Actinides and Rare Earths
Room Central Hall - Session AC-ThP

Actinides and Rare Earths Poster Session

AC-ThP-2 Nuclear Forensics, Fission Track Analysis , Star Segmentation and Classification Using Deep Learning, *N. Elgad, R. Babayew, Y. Yehuda-Zada,* Ben Gurion Uni., Israel*; J. Lorincik,* Research Centre Řež, Czechia*; M. Last, I. Orion, G. Katarivas-Levy,* Ben Gurion Uni., Israel*; A. Weiss,* Bar Ilan University, Israel*;* ***Itzhak Halevy****,* Ben Gurion Uni., Israel

A novel approach for identifying star shapes in microscopic images via deep learning segmentation and classification.

Semi-automated data tagging: Introducing a new method for labeling data.

U-Net FCN model: Designed for segmenting various star-like shapes in single or multi-class scenarios.

Identifying shapes under a microscope involves separating the sampling paper into ~10,000 images, akin to finding a needle in a haystack due to its grueling nature and human eye limitations.

Star identification has evolved from manual eye scans to recent advancements in automatic

image processing tools.

This work employs a deep learning model, specifically the U-Net network, for segmentation and classification, integrating a 5-fold cross-validation analysis.

Work Content:

1. A New image star database was created.
2. Characterization of star types, model architecture, and optimization.
3. Training for single and multi-class datasets.
4. Automation of segmentation for batches of images.
5. Research on optimizing frequency, epochs, and threshold settings,
6. collaborating on simulated star classification.

Model achieved 92.04% accuracy for small single-class stars (<60µm), with 0.84 ROC area.

Segmentation of dual-class stars reached 86.3% validation accuracy.

Identification of simulated stars with varying leaf counts achieved 82.63% accuracy, while a computational model for higher magnitude stars achieved 0.90 ROC area.

AC-ThP-3 Tracking the Impact of Varied Oxygen Partial Pressure during PLD Growth on the Magnetic Response of Metastable Orthoferrite $LuFeO_3$, ***Washat Ware****, M. Frye, M. Mourigal, L. Garten,* Georgia Institute of Technology, USA

While the orthorhombic phase of $LuFeO_3$ (o-LFO) has attracted attention as a potential defect-induced room temperature multiferroic[1], stabilizing this metastable phase while maintaining the correct defect concentrations remains a challenge. The antiferromagnetic behavior in o-LFO is thought to stem from a weak canted moment that is perpendicular to the c-axis, while ferroelectricity is attributed to anti-site defects.[1, 2] Given the sensitivity of this material to disorder and oxygen vacancies, it is critical to understand how processing affects the magnetic and ferroelectric phase transitions of this orthoferrite. Determining the magnetic phase transition temperatures and potential for ferroic coupling within o-LFO is the first step toward reaching the full potential of this material for magnetoelectric applications.

In this work, we characterize the impact of processing on the magnetic response of o-$LuFeO_3$ grown by pulsed laser deposition (PLD). A stoichiometric $LuFeO_3$ target was used to deposit thin films onto (100) $SrTiO_3$ substrates while varying either the oxygen partial pressure (p_{O2}), laser fluence, growth temperature, or growth rate. X-Ray diffraction (XRD) indicates that the metastable orthoferrite phase is stabilized with a solely (001) orientation under all conditions. Varying the oxygen partial pressure (p_{O2}) from 0.05 mbar to 0.2 mbar, leads to a broadening of the (001) family of peaks of the o-$LuFeO_3$, which could indicate a decrease in crystallite size, variation in orientation, or microstrain at the microscopic level. Varying laser fluences from 2 J/cm^2 - 2.2 J/cm^2 show a similar pattern of broadening but the effect is not as prominent. High temperature, vibrating sample magnetometry (VSM) is used to track the change in transition temperature under field cooling (FC) and zero field cooling (ZFC). Under FC and ZFC in the narrow field range, a phase transition is seen around 50 K and 270 K, and a clear magnetic hysteresis is present for all samples. Building the understanding of the magnetic phase transition in orthoferrite, $LuFeO_3$ is the first step towards developing room temperature magnetoelectric coupling devices.

1. Choo, E., Klyukin, K., Su, T. Kaczmarek, A., Ross, C. “Composition-Dependent Ferrolectricity of $LuFeO_3$ Orthoferrite Thin Films,” Adv. Electron. Mater. 2300059(*9*), 1-8 (**2023**).
2. Chowdhury, U. et al. “Origin of Ferroelectricity in orthorhombic $LuFeO_3$,” Phys. Rev. B. 100 (*11*), 1-11 (**2019**).

AC-ThP-4 Electronic Structure of a Nodal Line Semimetal Candidate, ***Iftakhar Bin Elius****,* University of Central Florida*; S. Regmi,* Idaho National Laboratory*; A. Sakhya,* University of Central Florida*; V. Buturlim,* Idaho National Laboratory*; M. Sprague, M. Mondal, N. Valadez,* University of Central Florida*; T. Romanova,* Polish Academy of Sciences, Poland*; A. Kumay,* University of Central Florida*; A. Ptok,* Polish Academy of Sciences, Poland*; K. Gofryk,* Idaho National Laboratory*; D. Kaczorowski,* polish academy of Sciences, Poland*; M. Neupane,* University of Central Florida

*Ln*SbTe (*Ln*= lanthanides) compounds isostructural to well-known ZrSiS family of nodal line semimetals offer a rich platform for studying topological features as well as interaction of topology, magnetism, and electronic correlation owing to the presence of 4f electrons. We performed systematic magnetic field induced thermal transport, temperature dependent magnetic susceptibility and field dependent magnetization studies of rare-earth based ternary semimetals of this seriesat low temperature. To investigate the electronic structure of the materials, angle resolved photoemission spectroscopy (ARPES) and first principles-based calculations were performed. Multiple nodal lines along Γ−X and Γ−M high symmetry directions were observed in photon energy dependent ARPES measurements. Our investigation indicates that this system can provide a rich platform to study the interplay of magnetism, topology and correlation.

AC-ThP-5 Grain Boundary and Heterointerface Structures and Defects in Pu Oxides: Classical Molecular Statics Study to Inform Further Ab Initio Investigation, ***Larissa Woryk****, R. Atta-Fynn, A. Kohnert, S. Hernandez,* Los Alamos National Laboratory

Plutonium metal forms a passivated oxide layer upon exposure to air, with varying stoichiometry depending on oxygen conditions. At lower temperatures, interfaces in oxides can facilitate corrosion via fast-transport pathways. This can result in further growth of the oxide layers, or of corrosion via other species, such as hydriding from the absorption and transport of hydrogen throughout the material. Any of these forms of corrosion can have implications on the stability and longevity of material in storage. Structural, defect, and transport properties can vary across different grain boundaries and heterointerface orientations. This study presents structures and associated energies of selected Pu_2O_3-PuO_2 interfaces and selected grain boundaries, calculated with molecular statics, along with associated defect structures and formation energies. Comparisons of interfacial energies can suggest which interfaces might be more prevalent in these materials, which could then play a larger role in influencing material properties and behavior. Comparisons of defect energies, both across different interfaces and between interfaces and in bulk, can suggest influence of interfaces in corrosion and in transport phenomena more broadly.

The Cooper-Rushton-Grimes interatomic potential will be utilized for the molecular statics calculations as it has demonstrated comparable values to experimental lattice and elastic constants, and thermal properties [1]. Where applicable, the modification to this potential to include Pu^{3+} is also included, as developed by Takoukam-Takoundjou, *et al* [2].

[1] M W D Cooper *et al* 2014 *J. Phys.: Condens. Matter* **26** 105401.

[2] C Takoukam-Takoundjou *et al* 2020 *J. Phys.: Condens. Matter* **32** 505702.

AC-ThP-6 Exploring the Combined Influence of Alpha Irradiation, Dissolved Hydrogen, and Palladium Addition on UO2 Corrosion Using a Microfluidic Electrochemical Cell, ***Jennifer Yao****, J. Heo, B. McNamara, E. Ilton, E. Buck,* PNNL

Understanding the influence of alpha irradiation and dissolved hydrogen on the corrosion behavior of uranium dioxide (UO_2) is essential for evaluating the long-term impacts on storage environments.[1] Traditional experiments involving bulk SNF are typically costly due to stringent requirements for radiation shielding. To address these challenges, we have developed a novel particle-attached microfluidic electrochemical cell (PAMEC). This innovative microfluidic technique enables the multimodal analysis of UO_2 corrosion

under simulated SNF storage conditions using minimal material quantities, significantly reducing both costs and risks of hazardous exposure.[2, 3]

Recently, we have incorporated palladium—a noble metal commonly found in irradiated nuclear fuel—into the UO_2 working electrode. This modification allows us to investigate how noble metals influence UO_2 degradation behavior in the presence of dissolved H_2 and alpha irradiation. In addition to utilizing electrochemical measurements such as open circuit potential, for qualitative insights into the degradation of the UO_2 matrix, PAMEC's unique design supports in situ chemical imaging of the UO_2 surface. In this study we employ in situ imaging of the PAMEC working electrode using scanning electron microscopy (SEM) combined with energy-dispersive X-ray spectroscopy (EDS). This integration of techniques offers a comprehensive view that enhances our understanding of the UO_2 corrosion mechanism. The potential applications of this technology are extensive, providing a safer and more effective alternative for conducting corrosion studies on materials that pose high exposure risks or are difficult to access due to their rarity.

References:

1. *Long-term storage of spent nuclear fuel.* Nature Materials, 2015. **14**(3): p. 252-257.
2. *A microfluidic electrochemical cell for studying the corrosion of uranium dioxide (UO(2)).* RSC Adv, 2022. **12**(30): p. 19350-19358.
3. *Advancing radioactive material research method: the development of a novel in situ particle-attached microfluidic electrochemical cell.* Frontiers in Nuclear Engineering, 2023. **2**.

Author Index

Bold page numbers indicate presenter