Thermal Energy Transport under Irradiation (TETI)
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Lead Institution: Idaho National Laboratory
Class: 2018 – 2022

Mission Statement*: To provide the foundational work necessary to accurately model and ultimately control electron- and phonon-mediated thermal transport in 5f-electron materials in extreme irradiation environments.*

To efficiently capture the energy of the nuclear bond, advanced nuclear reactor concepts aim to use fuels that must withstand unprecedented temperature and radiation extremes. In these advanced fuels, thermal energy transport under irradiation is directly related to reactor efficiency as well as reactor safety and is arguably one of the most important material properties. The science of thermal transport in nuclear fuel under irradiation is a grand challenge due to both computational and experimental complexities. In addition to accurately treating strong spin-orbit coupling of 5*f* electrons, the computation challenge also includes how to accurately model the formation of defects along with their influence on thermal transport.

The Center for Thermal Energy Transport under Irradiation ("Center" or "TETI") brings together an internationally recognized, multi-institutional team of experimentalist and computational materials theorists to develop a comprehensive, atom-to-mesoscale understanding of phonon and electron transport in advanced nuclear fuels. The Center takes a broad aim with two thrust areas: (1) phonon transport in advanced oxide fuels and (2) electron transport in advanced metallic fuels. The model fuels studied within the Center will be single crystal and polycrystalline thorium oxide and thorium oxide doped with uranium and the binary uranium-zirconium (UZr) system. This challenge is organized around a carefully constructed set of *science questions* that seek to close key knowledge gaps related to thermal energy transport in 5*f*-electron materials:

1. What is the impact of 5*f* electrons on phonon and electron structure in $Th_{1-x}U_xO_2$ and U-Zr alloys?
2. How do intrinsic and irradiation-induced defects self-organize in $Th_{1-x}U_xO_2$ and U-Zr alloys, and what are their impacts on electron and phonon scattering?
3. What are the collective effects of defects, defect ordering, and defect supersaturation on thermal transport $Th_{1-x}U_xO_2$ and U-Zr alloys?

Understanding electron- and phonon-transport characteristics from knowledge of chemistry / structure will have a far-reaching impact on materials development. Examples include utilization of defect organization under irradiation to improve thermal transport in advanced nuclear fuels, tailoring electron scattering in textured nanocrystals to enhance thermal conductivity of metal interconnects, simultaneously controlling electron and phonon transport in thermoelectric devices, and harnessing strong spin-orbit coupling to realize new paradigms for quantum materials.

Tackling the computational complexity is a far-reaching challenge. At the atomistic scale, the approach will involve using density functional theory plus dynamic mean field theory (DFT+DMFT) to understand the role of 5*f* electrons on phonon and electron transport, defect formation, and electron scattering mechanisms. At the mesoscopic-length scale, thermodynamic modeling and molecular dynamics will be used to understand defect interaction and evolution as well as phonon-scattering mechanisms. Also at this scale the Boltzmann transport equation (BTE) will be used to model transport.

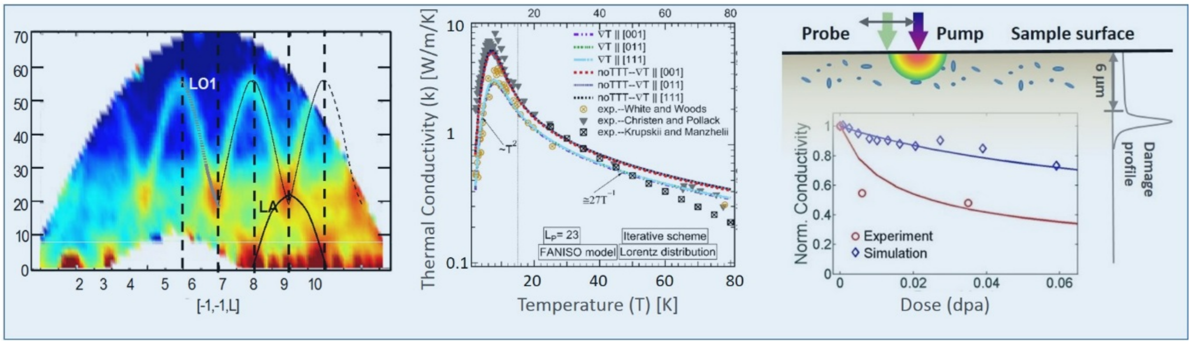

Figure. 1. *Left*: Dynamic structure of UO_2 measured along Q-[-1,-1,L] at 400k using the ARCS instrument at the Spallation Neutron Source, Oak Ridge National Laboratory. *Middle*: Simulation of the thermal conductivity of solid argon using the Boltzmann Transport Equation approach. *Right*: Time-resolved thermal wave measurement of conductivity in the plateau region of proton-irradiated UO_2 compared to MD simulation. These studies will be generalized to include both phonon and electron transport to investigate thermal transport in the $Th_{1-x}U_xO_2$ and UZr systems.

This modeling approach will be complemented by a well-defined set of electron- and phonon-structure measurements and transport measurements on ion-irradiated model fuels having well-characterized microstructures. Inelastic neutron scattering will be used to measure phonon dispersion and lifetime. Angularly resolved photoemission spectroscopy, and low-temperature magnetic field measurements (de Haas-van Alphen and Shubnikov-de Haas) will be used to obtain the electronic structure of metallic fuels. Thermal wave microscopy combined with coherent acoustic wave spectroscopy will be used to make spatially resolved thermal transport measurements across isolated grain boundaries and the damage plateau in ion-irradiated samples. The influence of supersaturation of point defects will be obtained by making first-of-its-kind in-reactor measurements of thermal conductivity.

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