Project Title

Thermal Conductivity in Metallic Fuels

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ABSTRACT:

Different alloying elements and impurities in metallic fuels systems such as U-Zr and Np-Zr strongly influence their thermal properties. It is therefore important to understand their effects on the thermal conductivity in order to control the operating temperature and consequently to improve the fuel performance. Such improvements will ultimately increase the lifetime of the fuel, improve the reactor efficiency, and reduce the amount of nuclear waste.

The goal of this proposal is to determine accurate thermal conductivity in U-Zr and Np-Zr fuel materials. In metal, the thermal conductivity is the sum of the electronic thermal conductivity κ_{el} and the lattice thermal conductivity κ_{ph}. The necessary electronic and phonon structure needed to predict κ_{el} and κ_{ph} will be predicted from density functional theory (DFT) calculations. We will then determine the corresponding transport properties using higher level kinetic models, namely the electrical part of the thermal conductivity using the BoltzTraP code and the lattice part of the thermal conductivity using the phonon Boltzmann transport equation.

The DFT-calculated thermal conductivities will be used as an input for the mesoscale simulation code called MARMOT, which will calculate the effective thermal conductivity of materials, considering microstructure effects. The effective thermal conductivity will be directly compared to experimental thermal conductivities using laser flash measurement at INL.

Experiments will have a key role in this study by validating the calculated effective thermal conductivity using the MARMOT code and by helping determing optimal DFT simulation parameters. Thus, the accuracy of our calculated thermal conductivity coming either from DFT calculations or the MARMOT code will require an iterative cycle that guides and informs experiment, simulation, and theory. From the theoretical results readjusted with the experimental data, we will request synthesis of new samples with concentration that will allow theorists to validate not only the calculated results but also the protocol used to calculate and extrapolate the theoretical thermal conductivity in metallic fuels. The proposed coupling between simulation and experiment are schematically represented in **Figure 1**. Using this coupling to calculate the thermal conductivity, we can understand the materials properties in a fast and efficient way, and work iteratively to improve the fuel lifetime by understanding its thermal behavior.

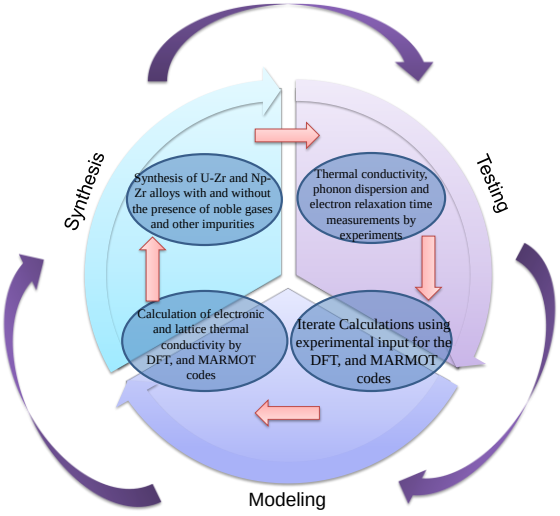

Fig. 1: Coupling between experiments, simulation, and theory