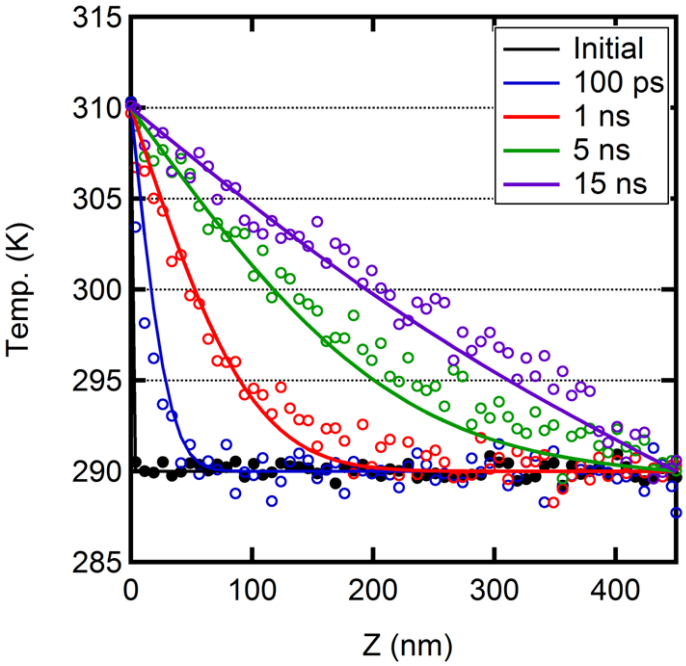
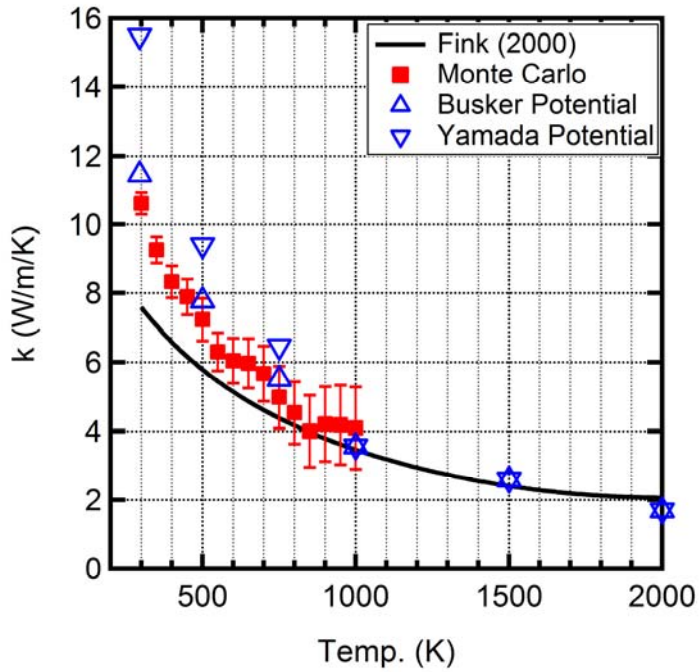
Highlight: Monte Carlo Simulations of Thermal Transport in UO_2





EFRC researchers Ryan Deskins (Ph.D. student) and Anter El-Azab (PI) at Purdue University have developed a model to simulate heat transfer in UO_2 crystals at the mesoscale. The model is based on Monte Carlo (MC) simulation of phonon transport single crystals based on Boltzmann Transport Equation (BTE). **Above (left):** The energy content within a 450 nm thick slab of UO_2 is tracked by the MC simulation scheme and the local temperature is plotted as a function of position and time. The stochastic solution (symbols) is compared with an analytical solution to the 1D heat equation, using thermal diffusivity measurements reported in a review by Fink (2000) for 95% dense UO_2. The results agree well with the analytical solution, except for a slightly higher rate of energy transport. This makes evident a higher conductivity within the MC model when compared to experiment. **Above (right):** The heat flux and the temperature gradient in the steady state are used to recover the conductivity of UO_2 crystal as a function of the (mean) temperature. The MC results approach that seen in experiments at higher temperatures. This trend is expected as conductivity becomes more and more dependent on intrinsic phonon scattering processes instead of boundary or impurity scatterings. It is expected that introducing defect phonon scatterings within our model will reduce our lower-temperature conductivities to be closer to experimental measurements. Incorporating defects into the phonon transport simulations is our next step.

This work has been presented at the 2011 MRS Fall Meeting in Boston, MA and also at the 2012 MRS Spring Meeting in San Francisco, CA. A manuscript is being prepared for submission to *Modelling and Simulation in Materials Science and Engineering*.