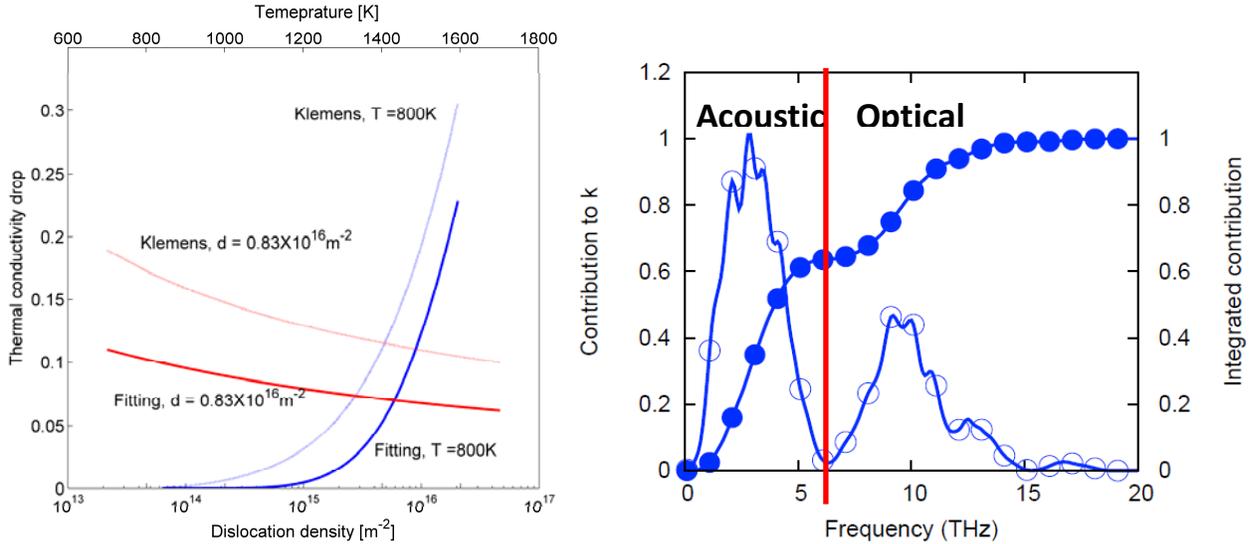


Highlight: Thermal Transport in UO_2 from Atomistic Simulations.



EFRC supported activities of computational materials science group in the University of Florida under guidance of Prof. **Simon Phillpot** (PI) include investigations of the intricate details of the thermal transport in the pure UO_2 using first principles methods and lattice dynamics (**Aleksandr Chernatynskiy**, Postdoc), studies of the thermal transport in UO_2 with microstructure (grain boundaries, dislocations) via molecular dynamics (MD) simulations (by **Bowen Deng**, Ph.D. student) and development of the COMB UO_2 potential (by **Yangzhong Li**, Ph.D. student).

Above (left): Thermal conductivity reduction as a function as a function of the dislocation density at fixed 800K (blue curves, bottom scale) and function of temperature at fixed density (red curves, upper scale). Bold curves are the results of the MD simulations, in comparison with the predictions of the Klemens model on the thermal transport. This is the first MD study of the dislocations effect on thermal conductivity in any material, and our investigations confirm that Klemens model provide satisfactory description of the effect. In the case of UO_2 it is important only at very high dislocation densities. This work is about to be submitted to the Journal of the Nuclear Materials.

Above (right): Spectral thermal conductivity in UO_2 as computed from first principles using lattice dynamics and Boltzmann Transport Equation formalism. Integrated contribution plot (right axis) shows that optical modes contribute nearly 40% percent of the overall thermal conductivity, an unusually high percentage. This result agrees very well with the inelastic neutron measurements performed at ORNL within this EFRC program and refutes previously published results that lack of optical phonons contribution is the cause of the small thermal conductivity in UO_2 . A joint publication is nearing submission.

These works have been presented at the 2011 MRS Fall Meeting in Boston, MA and TMS 2012 meeting in Orlando, FL.