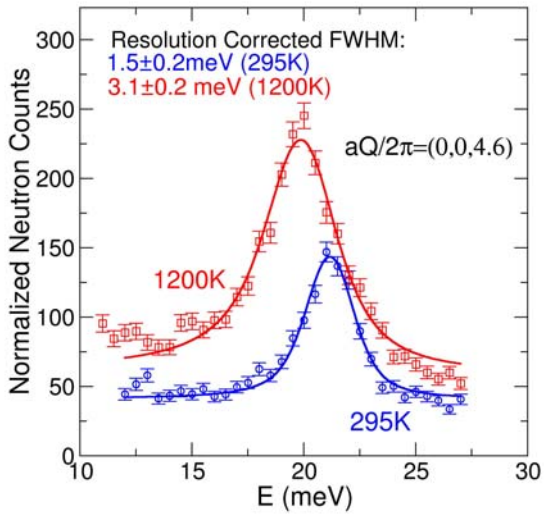
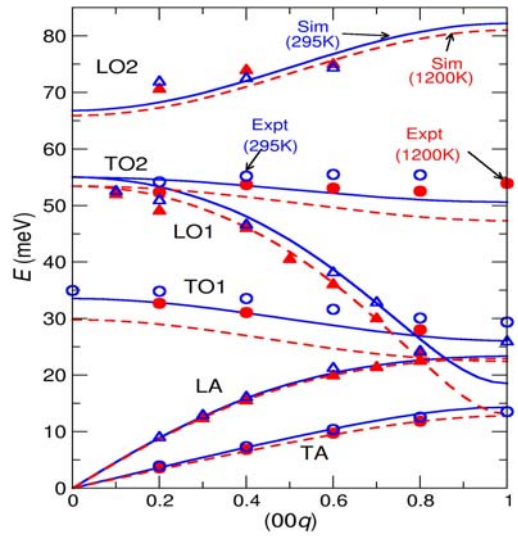
Highlight: inelastic neutron scattering study of phonon dynamics in UO_2 for comparison with theory and understanding thermal conductivity



Phonon spectra for a longitudinal acoustic (LA) phonons measured at 295 K and 1200 K using inelastic neutron scattering for the determination of phonon energy and linewidth.



Phonon dispersion curves for UO_2 along [001] measured by inelastic neutron scattering (blue and red symbols) compared with Catlow shell model lattice dynamics simulations (blue solid and red dotted lines) at 295 K and 1200 K.

Judy Pang (ORNL), **Bill Buyers** (NRC, Canada) and **Ben Larson** (ORNL) have performed extensive samplings of phonon energies and phonon linewidths in single crystal UO_2 using inelastic neutron scattering to determine the impact of anharmonicity on thermal conductivity (left panel). Phonon measurements at 295 K and 1200 K as a function of phonon branch and wavevector for the three high symmetry directions have made it possible to determine experimentally the contribution of thermal conductivity for individual phonon branches and temperatures. The phonon dispersion and linewidth measurements provide a direct test of lattice dynamics simulations by EFRC researchers A. Chernatynskiy and S.R. Phillpot at UF using the Catlow shell model (right panel) and first principles simulations (not shown). The phonon lifetime measurements also provide experimental input for the development of thermal conductivity models for UO_2 based on the Boltzmann transport equation that are being performed by EFRC researchers R. Deskins and A. El-Azab at Purdue University.

This work has been presented at the 2011 MRS Fall Meeting in Boston, MA