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Phonon lifetime investigation of anharmonicity and thermal conductivity in UO_2[1] JUDY PANG, Oak Ridge National Laboratory, ALEKSANDR CHERNATYNSKIY, University of Florida, WILLIAM BUYERS, National Research Council, Canada, BENNETT LARSON, Oak Ridge National Laboratory, SIMON PHILLPOT, University of Florida — Understanding low thermal conductivity in UO_2 requires a correct accounting for anharmonic phonon-phonon scattering processes. However, over the last five decades there have been remarkably few high-temperature studies of phonon processes in UO_2 to underpin its widespread use as a reactor fuel. We have used high-resolution inelastic neutron scattering measurements of individual phonon lifetimes (linewidths) and dispersion at 295 and 1200 K to probe anharmonicity and thermal conductivity in UO_2 for individual phonon branches. We found that phonon lifetimes depend strongly on the phonon wave vector and that longitudinal optic phonon modes transport the largest amount of heat, in contrast to recent first principles simulations. The total thermal conductivities calculated using our phonon data demonstrate a quantitative correspondence between microscopic and macroscopic phonon physics. We have also performed density functional theory simulations showing semi-quantitative agreement with phonon lifetimes at 295 K, but larger anharmonicity than measured at 1200 K. These measured phonon dispersion and lifetimes form a benchmark dataset against which numerical simulations including anharmonicity may be assessed.

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