Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Phonon Anharmonicity in Silicon from 100 to 1500 K DENNIS KIM, H.L. SMITH, California Institute of Technology, Department of Applied Physics and Materials Science, J.L. NIEDZIELA, Instrument and Source Division, Oak Ridge National Laboratory, C.W. LI, Materials Science and Technology Division, Oak Ridge National Laboratory, D.L. ABERNATHY, Quantum Condensed Matter Division, Oak Ridge National Laboratory, B. FULTZ, California Institute of Technology, Department of Applied Physics and Materials Science — Silicon has widespread use in modern technology and understanding the thermodynamics and thermal transport is of great importance. As the phonons dominate the total entropy as well as thermal transport properties, it is essential to measure accurately the temperature-dependent lattice dynamics. Inelastic neutron scattering measurements of silicon were performed at temperatures ranging from 100 to 1500 K (previous neutron measurements of phonon dispersions of pure silicon extended only up to 700 K). The experiments were done on high-quality powder and on single crystals, which were shaped for optimal neutronics in the ARCS spectrometer at the SNS. Large phonon anharmonicities manifested by phonon energy shifts and broadenings at high temperatures were observed in measured phonon dispersions, and in the phonon density of states. At 1500 K the anharmonicity contributes approximately 80% of the deviation from the harmonic vibrational entropy. These large effects are beyond the predictions of the quasiharmonic model and demonstrate that phonon anharmonicity is a major contributor to both vibrational entropy and phonon lifetimes.

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Date submitted: 14 Nov 2014 Electronic form version 1.4