Abstract Submitted
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Phonon densities of states of Sn to 64 GPa[1] E.A. TANIS, C. CHEN, H. GIEFERS, X. KE, M. NICOL, M. PRAVICA, University of Nevada Las Vegas, E. ALP, J. ZHAO, Advanced Photon Source, C. GREFF, S. RUDIN, Los Alamos National Laboratory, W. PRAVICA, Wilber Wright College — We measured lattice dynamics of 3 phases of Sn to 64 GPa at ambient temperature by NRIXS and compare the results with DFT computations using the direct force method and all-electron PAW method as implemented in the VASP code. Calculations with either GGA or LDA approximations gave similar results. Other properties calculated from the results include: the Lamb-Mossbauer factor; the mean force constant; vibrational contributions to the Helmholtz free energy; the high and low temperature Debye temperatures; the Debye average phonon velocity; and the Debye-Gruneisen parameter. At all pressures, experimental and theoretical DOS agree well.

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