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Role of anharmonicity in the phonon contribution to the Grüneisen parameter R. RAVELO, University of Texas, El Paso, TX, B.L. HOLIAN, Los Alamos National Laboratory, Los Alamos, NM — The Grüneisen parameter γ is directly related to the thermal expansion of a solid and to its equation of state (EOS). Several formulations of γ based on the isothermal EOS and pressure derivatives of elastic moduli have been developed over the years and predict different values for γ at zero pressure and its pressure dependence. The uncertainty in these "mechanical" models can be addressed by density functional theory (DFT) calculations using the Mie-Grüneisen formulation in which the vibrational contribution to the pressure is treated within the quasi-harmonic approximation while the static contribution is accounted by the cold curve. However, the vibrational Grüneisen need not agree with either the thermodynamic value or any of the mechanical models, and is in fact overestimated in transition metals. We examine the difference between the vibrational and thermodynamic Grüneisen parameter employing both classical molecular dynamics and lattice dynamics and utilizing classical interatomic potentials for bcc and fcc crystals constructed to have similar elastic moduli and cold curves but with different degrees of anharmonicity and transverse and longitudinal Brillouin edge zone phonon frequencies.

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