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Pressure dependence of lattice anharmonicity and phonon lifetime in MgO: a first-principles calculation and implications for lattice thermal conductivity XIAOLI TANG, JIANJUN DONG, Auburn University — We report a recent first principles calculation of harmonic and anharmonic lattice dynamics of MgO. The 2^{nd} order harmonic and 3^{rd} order anharmonic interatomic interaction terms are computed explicitly, and their pressure dependences are discussed. The phonon mode Grüneisen parameters derived based on our calculated 3^{rd} lattice anharmonicity are in good agreement with those estimated using the finite difference method. The phonon lifetime due to lattice anharmonicity is calculated based on the single mode excitation approximation (SMEA). We have further estimated the isotope effect on phonon lifetime within the random mass disorder approximation. The implications for lattice thermal conductivity at high pressure are discussed based on a simple kinetic transport theory.

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