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First-principles study of phonon-phonon interaction in FCC metals at high temperatures XIAOLI TANG, CHEN W. LI, Department of Material Science and Applied Physics, California Institute of Technology, BRENT FULTZ, Material Science and Applied Physics, California Institute of Technology — Third-order lattice anharmonicity induced phonon broadening of FCC metals (including Al and noble metals Cu, Ag, Au) were calculated from first-principles density functional theory (DFT) using the second-order perturbation theory, where anharmonic force constants were obtained from supercell finite displacement method combined with DFT calculations. For aluminum, the good agreement between our calculations and prior measurement of phonon linewidth at 300K and our new measurement of phonon density of states to 750K indicates the third-order phonon-phonon interactions can account for the lifetime broadenings of phonons in aluminum to at least 80% of its melting temperature. A systematic study of noble metals further suggests that, despite of the similarity among these systems, scattering kinematics play an important role in determining the relative anharmonicity between the modes, while potential anharmonicity modulates the absolute phonon decay rate.

Xiaoli Tang
Department of Material Science and Applied Physics,
California Institute of Technology

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