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Phonon Engineering in Metals from First Principles NICHOLAS LANZILLO, J. THOMAS, E.B. WATSON, M. WASHINGTON, SAROJ K. NAYAK, Rensselaer Polytechnic Institute — The electron-phonon interaction in metallic systems controls the electronic transport properties, including both electrical and thermal resistivity. The effect of compressive strain on the electron-phonon interaction in metals is investigated using first-principles density functional theory, and we propose various ways to "engineer" this interaction for various technological applications. In particular, we show that by applying compressive strain on the FCC crystals of Al, Cu, Ag and Au, the net electron-phonon scattering rate decreases and likewise the electrical resistivity decreases with increasing pressure. This trend is corroborated by experimental measurements of the resistance of a 0.5 mm diameter high-purity Al wire pressurized up to 2 GPa in a solid-media pressure apparatus at room temperature. The rate of the decrease in electrical resistivity as a function of pressure as determined by experiment is matched by the rate predicted by theory. Our simulations show that Al nanowires have the same response to strain as the bulk crystal; the net electron-phonon scattering can be reduced through compressive strain. Modifying the electron-phonon interaction in metallic structures shows great promise for future nano-electronic devices.

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