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Nanophononic metamaterial: Thermal conductivity reduction by dispersion-resonance hybridization MAHMOUD I. HUSSEIN, HOSSEIN HONARVAR, LINA YANG, University of Colorado Boulder — Engineered manipulation of phonons can yield beneficial thermal properties in semiconducting materials. One pivotal application relates to thermoelectric materials, or the concept of converting energy in the form of heat into electricity and vice-versa. The ability to use nanostructuring to reduce the thermal conductivity without negatively impacting the power factor provides a promising avenue for achieving high values of the thermoelectric energy conversion figure-of-merit, ZT. In this work, we propose a novel nanostructured material configuration that seeks to achieve this goal. Termed "nanophononic metamaterial," the configuration is based on a silicon thin-film with a periodic array of pillars erected on one or two of the free surfaces. The pillars qualitatively alter the base thin-film phonon spectrum due to a hybridization mechanism between their local resonances and the underlying atomic lattice dispersion. Using lattice dynamics calculations and molecular dynamics simulations, we predict a drop in the thermal conductivity to as low as 50% of the corresponding uniform thin-film value despite the fact that the pillars add more phonon modes to the spectrum.

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