

# Propagation Characteristics of Narrowband Thermal Phonons Under Atomic-scale Local Resonance Conditions

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Thermal energy conduction in nanostructures involves various atomic-scale phonon mechanisms with a complex interplay between wavelike and particle behavior. In nanoscale configurations where the feature sizes are smaller or on the order of the phonon mean free path, it is possible to engineer the wavelike behavior to, for example, impede heat conduction—which is favorable for thermoelectric energy conversion. While reducing the dimensionality or introducing obstacles to the heat flow in nanostructures can reduce the thermal conductivity [1], it can also impede the power factor thus negating any substantial increase in the thermoelectric figure of merit  $ZT$ . Control of wave phenomenon in the sub-phonon mean free path regime, on the other hand, offers the potential to improve  $ZT$ . One approach involves the introduction of resonating substructures to a conventional material, such as silicon, to form a *nanophononic metamaterial* (NPM) [2]. These substructures create standing phonon waves that couple with the underlying propagating phonons causing a significant modification of the dispersion relation, including substantial reduction in the phonon group velocities and the creation of mode localizations. This ultimately decreases the lattice thermal conductivity—all without affecting the electronic properties [3].

In this work, we use narrowband wave-packet excitations to investigate the impact of local resonances on room temperature phonon transport in NPMs in the form of nanopillared membranes and compare with corresponding nanostructures that do not include local resonances. Our results provide an in-depth analysis and elucidation of the underlying phonon localization effects associated with the local resonances. By controlling the wave-packet frequency, we are able to isolate the role of the local resonances on the thermal energy propagation from other effects that also influence the total lattice thermal conductivity such as phonon-boundary scattering. These observations open promising new possibilities for experiments to further unlock the potential of atomic-scale local resonances.

## References

1. D. Li, Y. Wu, P. Kim, L. Shi, P. Yang, and A. Majumdar, *Appl. Phys. Lett.* **83**, 2934-2936, (2003).
2. B.L. Davis and M.I. Hussein, *Phys. Rev. Lett.* **112**, 055505, (2014).
3. B.T. Spann, J.C. Weber, M.D. Brubaker, T.E. Harvey, L. Yang, H. Honarvar, C.-N. Tsai, A.C. Treglia, M. Lee, M.I. Hussein, and K.A. Bertness, *Adv. Mater.* **35**, 2209779 (2023).