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Resonant thermal transport and potential impact on thermoelectric energy conversion

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Thermoelectric materials convert heat into electricity or vice versa through a solid-state process. For the conversion efficiency to be competitive with fluid-based technologies, a thermoelectric material must be a good insulator of heat while, simultaneously, exhibit good electrical properties–a combination that is hard to find in common materials. Here we present the concept of a locally resonant *nanophononic metamaterial* (NPM) [1-3] to overcome this natural trade-off in properties. One realization of an NPM is a freestanding silicon membrane (thin film) with a periodic array of nanoscale pillars standing on one or both free surfaces. Heat is transported along the membrane portion of this nanostructured material as a succession of propagating vibrational waves, *phonons*. The atoms making up the minuscule pillars on their part generate resonant vibrational waves, which we describe as *vibrons*. The vibrons represent new modes added to the system. These two types of waves interact causing a mode coupling for each pair which appears as an avoided crossing in the pillared membrane's phonon band structure. This in turn (1) reduces the base membrane phonon group velocities around the coupling regions, and (2) enables mode localization in the nanopillar portions. These two effects bring rise to a unique form of conductive transport through the base membrane, namely, *resonant thermal transport*. The in-plane thermal conductivity decreases as a result. Given that the number of vibrons scales with the number of degrees of freedom of a nanopillar, this effect intensifies as the size of the nanopillar(s) increases, and in principle may be tuned to influence the entire phonon spectrum (which for silicon extends up to over 17 THz). This novel phenomenon thus provides an opportunity for achieving exceptionally strong reductions in the thermal conductivity. Furthermore, since the mechanisms concerned with the generation and carrying of electrical charge are practically independent of the phonon-vibron couplings, the Seebeck coefficient and the electrical conductivity are at most only mildly affected, if not at all.

In this talk, I will introduce the concept of an NMP and present its phonon properties using lattice-dynamics calculations and its thermal conductivity using molecular dynamics simulations. Preliminary electrical properties predictions using density functional theory will also be presented, as well as preliminary experimental results and plans for integration into practical device architectures. Finally, projections of record-breaking values of the thermoelectric energy conversion figure of merit *ZT* will be provided.

Given the relatively large size of our unit-cell modes, I will also overview–if time permits–a Bloch-mode substructuring technique we developed to speed up phonon and electron band structure calculations [4].

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[3] Honarvar, H. and Hussein, M.I., *Phys. Rev. B.* **97**, 195413, 2018.
[4] Krattiger, D. and Hussein, M.I., *J. Comput. Phys.* **357**, 183-205, 2018.

Short Bio: Mahmoud I. Hussein is an Associate Professor and the Alvah and Harriet Hovlid Professor at the Department of Aerospace Engineering Sciences at the University of Colorado Boulder. He also holds a faculty affiliate appointment at the Department of Applied Mathematics, and serves as the Faculty Director of the Pre-Engineering Program at the College of Engineering and Applied Science. He received a BS degree from the American University in Cairo (1994) and MS degrees from Imperial College, London (1995) and the University of Michigan–Ann Arbor (1999, 2002). In 2004, he received a PhD degree from the University of Michigan, after which he spent two years at the University of Cambridge as a postdoctoral research associate.

Dr. Hussein's research focuses on the dynamics and physics of materials and structures, especially phononic crystals and locally resonant phononic metamaterials, at both the continuum and atomistic scales. His approach to phononics is rather broad ranging from vibrations of aerospace structures to lattice dynamics and thermal transport in silicon-based nanostructured materials. His studies are concerned with physical phenomena governing these systems, relevant theoretical treatments, and analysis of the effects of dispersion, resonance, dissipation and nonlinearity. He also develops techniques for fast band-structure calculations.

Dr. Hussein received a DARPA Young Faculty Award in 2011, an NSF CAREER award in 2013, and in 2017 was honored with a Provost's Faculty Achievement Award for Tenured Faculty at CU Boulder. He has co-edited a book titled *Dynamics of Lattice Materials* published by Wiley. He is a Fellow of ASME and an associate editor for the *ASME Journal of Vibration and Acoustics*. In addition, he is the founding vice president of the International Phononics Society and has co-established the Phononics 20xx conference series which is widely viewed as the world's premier event in the emerging field of phononics.