Large-scale vibron-phonon couplings: A strategy for raising the thermoelectric figure-of-merit

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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) [1-4] 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 erected on one or both free surfaces. Heat is transported along the membrane portion of this nanostructured material as a succession of wavenumber-dependent propagating vibrational waves, *phonons*. The atoms making up the minuscule pillars on their part generate wavenumber-independent resonant vibrational waves, which we describe as *vibrons*. These two types of waves linearly 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) enables the generation of new modes localized in the nanopillar portion(s) and (2) reduces the base membrane phonon group velocities around the coupling regions. In addition, the phonon lifetimes drop due to changes in the scattering environment, including both phonon-phonon scattering and boundary scattering.

These effects bring rise to a unique form of 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, these effects intensify as the size of the nanopillar(s) increases–possibly reaching millions of vibrons–up to the limits of the phononic mean-free-path distribution. In principle, the vibron density of states may be tuned to conform with that of the phonons across 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 thermal conductivity predictions using lattice-dynamics-based calculations and molecular dynamics simulations, as well as preliminary electrical properties predictions using density functional theory. Some early experimental results will be presented as well. In conclusion, projections of record-breaking values of the thermoelectric energy conversion figure of merit *ZT* will be provided.

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[4] Hussein, M.I., Tsai, C.N. and Honarvar, H., "Thermal conductivity reduction in a nanophononic metamaterial versus a nanophononic crystal: Review and Comparative Analysis," *Advanced Functional Mater*ials **30**, 1906718, 2020.

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Bio: Mahmoud I. Hussein is the Alvah and Harriet Hovlid Professor in the Smead Department of Aerospace Engineering Sciences, and has a courtesy and affiliate faculty appointments in the Departments of Physics and Applied Mathematics, respectively, at the University of Colorado Boulder. He is the director of the Pre-Engineering Program at the College of Engineering and Applied Science, and the director of the Phononics Laboratory. He received a BS degree from the American University in Cairo and MS degrees from Imperial College, London and the University of Michigan–Ann Arbor. He earned his PhD from the University of Michigan in 2004, and completed postdoctoral research at the University of Cambridge from 2005-2007. 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 is a Fellow of ASME. 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. Dr. Hussein's research interests lie broadly in the fields of phononics and nonlinear wave propagation.