Phononics at the macroscopic and microscopic scales: Recent advances in complex band-structure engineering and atomic-scale resonant thermal transport

Mahmoud I. Hussein

Alvah and Harriet Hovlid Professor
Ann & H.J. Smead Department of Aerospace Engineering Sciences
Department of Physics
University of Colorado Boulder, USA

Phononics is an emerging field that seeks to elucidate the nature of intrinsic mechanical motion in both conventional and artificially structured materials, and use this knowledge to extend the boundaries of physical response at either the material or structural/device level or both. The field targets primarily acoustic, elastic, and/or thermal properties and usually involves the investigation and utilization of complex wave mechanisms encompassing one or more of a diverse range of phenomena such as dispersion, resonances, dissipation, and nonlinear interactions. The field bridges multiple disciplines across applied physics and engineering, and spans multiple scales reaching the atomic scale where a rigorous definition of phonons resides– quanta of lattice vibrations.

At the mascroscale, the mechanisms of local resonance [1] and inertial amplification [2] have been introduced intrinsically in material systems to form metamaterials with salient subwavelength band-gap properties. I will demonstrate how explicitly combining these two concepts within a single framework enriches not only the real part of the elastic band structure, but also both the imaginary wavenumber and imaginary frequency parts. The imaginary wavenumber response will be shown to produce low-frequency bounded stop bands with both strong and broadband spatial attenuation properties. Simultaneously, the imaginary frequency part of the spectrum will be seen to exhibit either enhanced or diminished dissipation, demonstrating unique temporal attenuation properties.

At the microscale, I will present the concept of a locally resonant *nanophononic metamaterial* (NPM) [3], of which one realization is a freestanding silicon membrane (thin film) with a periodic array of nanoscale pillars extruding out of 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. I will introduce the concept of an NMP and present thermal conductivity predictions using lattice-dynamics calculations and molecular dynamics simulations. Finally, the potential for this concept to produce high-efficiency thermoelectric energy conversion will be discussed and demonstrated.

[1] Liu, Z., Zhang, X., Mao, Y., Zhu, Y. Y., Yang, Z., Chan, C. T., and Sheng, P., "Locally resonant sonic materials," *Science* **289**, 1734–6, 2000.

[2] Yilmaz, C., Hulbert, G.M., and Kikuchi, N. "Phononic band gaps induced by inertial amplification in periodic media. *Phys. Rev. B* **76**, 54309, 2007.

[3] Davis, B.L. and Hussein, M.I., "Nanophononic metamaterial: Thermal conductivity reduction by local resonance," *Phys. Rev. Lett.* **112**, 055505, 2014.

Mahmoud I. Hussein

Alvah and Harriet Hovlid Professor
Smead Department of Aerospace Engineering Sciences
Department of Physics (Courtesy)
University of Colorado Boulder

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.