Understanding Phonon Transport Using Lattice Dynamics and Molecular Dynamics

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The conventional view and understanding of phonon transport, both through materials and at interfaces, is based on what is termed the phonon gas model (PGM). The PGM essentially treats the energy of phonons as analogous to gas particles that scatter from each other, boundaries or other imperfections in the system. This approach then hinges on the idea that every phonon has a well-defined velocity, which in turn is only well-defined if the atomic arrangement is periodic. However, phonons exist more generally in any system that consists of a macroscopically rigid body, where all the atoms vibrate around their respective equilibrium sites. This includes, not only pure homogenous crystalline materials, for which the PGM exhibits excellent agreement and is well founded, but also alloys (both ordered and disordered), amorphous materials and individual rigid molecules. The problem is then that the PGM is not well founded for these non-periodic systems. As a result, there is a lack of understanding of the underlying physics at play in systems where the atomic arrangement is non-periodic. In this respect, there is an alternative view of phonon transport that has gained traction over the last two decades, that is based on the fluctuation dissipation theorem, whereby phonon contributions to transport are assessed by the degree to which they are correlated, rather than the degree to which they scatter. A correlation based view of phonon transport has the potential to be more general and fill in the gaps of understanding associated with the PGM. This tutorial lecture will briefly overview the PGM but will go in depth on explaining the correlation based perspective of phonon transport. The lecture will discuss the usage of lattice dynamics and molecular dynamics to evaluate phonon contributions to transport, thereby providing a robust framework for understanding it.