Phonon modes in disordered systems

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Phonons govern a wide range of phenomena ranging from phase change to mechanical behavior and heat transport. They are characterized by the normal modes of vibrations, which are non-interacting collective excitations of atomic vibrations. Phonon modes and the corresponding dispersion relationships are typically evaluated by solving the dynamical matrix. This approach fails for disordered solids when there is a complete breakdown of translational symmetry even when there are well-identifiable dispersion relationships for such systems (from the density or longitudinal current fluctuations). In this work, we propose a new approach that makes use of the spatial Fourier component of the particle current to obtain the dispersion relationship without directly working with the dynamical matrix. First, we demonstrate that by Taylor expanding the particle current with respect to the atomic displacements and without invoking a repeating unit cell, the leading term corresponds to the normal modes of vibration. We then show that the key to extracting the phonon dispersion is to use eigen projections of the atom types in a multi-atom system.

Using atomistic simulations, we verify our approach on simple systems and then compute the dispersion relationships in glassy and radiation-damaged graphite systems. A glassy state is prepared by rapidly quenching a liquid (modeling using a binary Lennard-Jones potential) to low temperatures. The disordered state is confirmed through the radial distribution function and through the lack of long-range order. The radiation-damaged graphite system is prepared through large scale non-equilibrium cascade simulations. The carbon-carbon interaction is modeled using the Tersoff potential, which is additionally stitched with a Ziegler-Biersack-Littmark screened Coulombic potential. After equilibration, a primary knock-on atom that is placed at the center of the simulation box receives excess momentum along a certain specified direction. This initially creates a transient liquid-like state, which condenses to a solid state with a number of quasi-stable atomic scale defects following a ultra-rapid cooldown phase. We apply our methodology to both the glassy and radiation-induced disordered systems and compute their respective phonon dispersion relationships. Finally, we show how our approach can be generalized to extract the dispersion relationships corresponding to all the hydrodynamic variables including density, momentum and energy.