Abstract

"Phononic crystals are artificially engineered materials that can forbid phonon propagation in a specific frequency range that is referred to as a "phononic band gap." Phononic crystals that have band gaps in the GHz to THz range can potentially enable sophisticated control over thermal transport with "phononic devices." Control in this frequency range can also enable advancements in other fields such as optomechanical devices. Calculations of the phononic band diagram are the standard method of determining if a given phononic crystal structure has a band gap, and if so, what is that band gap's center frequency and width. However, calculating the phononic band diagram is a computationally expensive and time-consuming process that can require sophisticated modeling and coding. In addition to this computational burden, the inverse process of designing a phononic crystal with a specific band gap center frequency and width is a challenging problem that requires extensive trial-and-error work. In this dissertation, I first present colloidal nanocrystal superlattices as a new class of three-dimensional phononic crystals with periodicity in the sub-20 nm size regime. The phononic band diagrams of these superlattices were calculated using the plane wave expansion method. These calculations show that colloidal nanocrystal superlattices should possess phononic band gaps with center frequencies in the 10^2 GHz range and widths in the 10^1 GHz range. Varying the colloidal nanocrystal size and composition provides additional opportunities to fine-tune the phononic band gap. These predicted phononic band gap center frequencies and widths far exceed those in current experimental demonstrations of three-dimensional phononic crystals. These frequencies also create unique opportunities for phonon-photon interactions. This suggests that colloidal nanocrystal superlattices are a promising platform for the creation of high frequency phononic crystals. For the next topic, I explore opportunities to use machine learning for expedited discovery of phononic band gap presence, center frequency and width. To demonstrate this possibility, I calculate the band diagrams for over 14,000 two-dimensional phononic crystal structures and use the corresponding results to train and test various machine learning algorithms. While 14,000 band diagrams is a large number, it is important to note that this number is small when compared to the infinite number of phononic crystal structure possibilities. The best trained model predicts band gap formation (a classification problem) with 94% accuracy. It is also able to predict band gap center frequencies and band gap widths with coefficients of determination (R^2) values of 0.66 and 0.83, respectively. I also show that training the machine learning models with 5,000 samples yielded results that were nearly as good as the 14,000 samples. Moreover, training the models with just 500 samples still yielded algorithms with predictive value. Given a suitable data set with which to train machine learning models, this approach represents a vastly decreased computational-cost and time-burden for phononic crystal band gap discovery. This approach also lowers the coding and modeling requirements for determining phononic band gap presence, center frequency, and width. Lastly, I expand the above machine learning approach to tackle the inverse problem of phononic crystal design. Rather than determine phononic band gap properties for a given phononic crystal structure, I use machine learning to design a phononic crystal for a given set of phononic band gap properties. The best model involved a novel approach to identifying phononic crystal material-geometric properties, and could predict elastic modulus of host and inclusion, density of host and inclusion, and diameter-to-lattice constant ratio for target center and width frequencies with coefficients of determinations of 0.94, 0.98, 0.94, 0.71, and 0.94 respectively. The high values coefficients of determination represents great opportunity for phononic crystal design."