Fast Approximation of Phonon Density of States in Silicon Nanoclusters

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We approximate the phonon density of states in a cluster of 512 silicon atoms using a state extracted from a larger 2048 atom configuration. In reciprocal space two methods created distributions which produce energy-temperature curves on a similar order to that of the actual material: a genetic algorithm searching the entire space of possible frequency combinations was slightly outperformed by a calculation which assumes good acoustic behavior in the phonon modes. Both methods improve on results from real-space calculations but overestimate the prevalence of higher frequency phonons. We also consider the benefits of these methods over traditional calculations with respect to scaling and parallelization.