Abstract Submitted
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Vibrational Properties of Phononic Crystals[1] RALF MEYER, Laurentian University — Phononic crystals are periodically structured, artificial materials that use Bragg reflection to manipulate the propagation of elastic waves. It has been shown theoretically and experimentally that nanoscale phononic crystals can have significantly reduced thermal conductivities. This makes them candidates for thermoelectric materials with high figures of merit ZT and has generated interest in the properties of thermal phonons in these materials. In this work, the vibrational properties of nanoscale silicon phononic crystals are studied with molecular dynamics simulations as well as finite element method calculations. The molecular dynamics simulations account automatically for surface and interface effects that are important on the nanoscale. Comparison of the vibrational band structures makes it therefore possible to improve the computationally less demanding finite element model. Results are presented that show the character of the lowest non-acoustic bands and how the acoustic modes of the phononic crystal deviate from the bulk behavior for shorter wavelength. It is found that close to the Brillouin zone boundary a decoupling of the vibrations occurs in the phononic crystal.

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