Vibrational Modes and Optical Phonon Dispersion in Silicon Metalattices

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Abstract

Phonons underlie the propagation of sound and the transport of heat in materials. With outstanding progress in the design of phononic crystals, it is now feasible to control the acoustic properties of these materials and to endow them with unique acoustic properties. For instance, it has been shown that by decreasing the characteristic dimensions of a phononic crystal, the ability to control the frequency-dependent wave propagation of acoustic waves can be significantly enhanced. Recently, the successful fabrication of silicon metalattices — a silicon structure with a periodic array of nanopores — has opened up the possibility to effectively reduce the transport of heat in silicon. In addition, since the periodicity of these nanoporous structures is comparable to the wavelength of light, it is expected that they can provide a means to tune the optical properties of materials. We have calculated the vibrational modes of silicon metalattices using COMSOL Multiphysics® software. By applying adequate boundary conditions with the optical elastic constants computed from first principles, we have determined the optical phonon dispersion spectrum of silicon metalattices in remarkable agreement with atomistic models. Those results open up the possibilities to efficiently predict the influence of nanoscale geometry on the optical response of silicon metalattices.

Figures used in the abstract

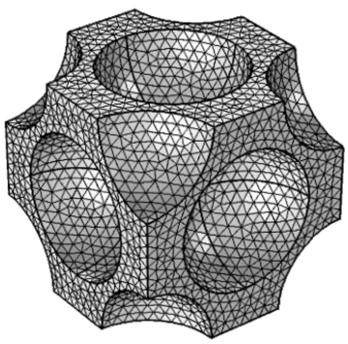

Figure 1: A silicon metalattice with a face-centered cubic arrangement of spherical nanopores.

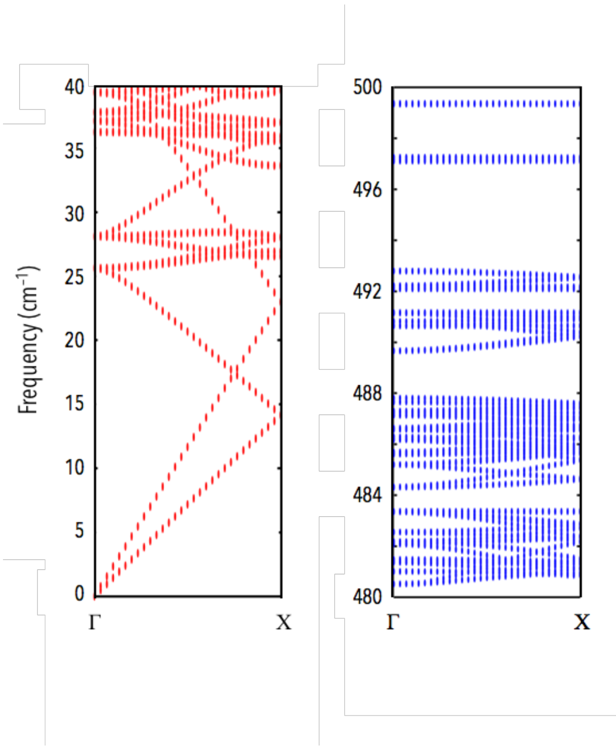

Figure 2: Acoustic and optical phonon spectra of silicon metalattice along the high-symmetry X direction.