Phonons dispersion curves And Phonons density of dielectric materials.

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Abstract

In this paper we present a theoretical study based on the vibrational properties of crystal lattices; such as diamond, silicon and germanium. A detailed calculation has been made to determine the dynamic matrices of these lattices. The phonon dispersion curves presented in this work concern the acoustic and optical modes propagating in the ΓX, ΓK and ΓL directions of the Brillouin zone (3D). In order to determine these dispersion curves we used the Born-von Karman model with the approximation of the central forces between the first and second neighbors. The radial and angular force constants were determined by fitting on experimental data using the generalised least squares method. This approach allows to determine the interaction parameters and the vibrational properties for each of the materials studied.

The phonon densities of FCC crystal lattices have been calculated by integration on phonons described by wave vectors of the first Brillouin zone. For this purpose, we used the Born-von Kàrmàn model with central forces between first and second neighbors. The values of the radial and angular force constants were determined by adjustment on the experimental dispersion curves. Our goal is to compare the phonon density spectra of FCC metals, and those of FCC dielectrics. For instance, we compare in this paper the calculated phonon spectra for copper, diamond, silicon, and germanium. These four materials are described by FCC crystal lattices, with one atom per unit cell for copper and two atoms per unit cell for the other three elements.

*Key words: phonons, dielectrics, metals, crystal lattice, dispersion curves, phonon density, force constants, vibrational properties*

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