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Temperature-enhanced far-infrared absorption in GaAs and GaP

HADLEY M. LAWLER, University of Maryland, ERIC L. SHIRLEY, NIST, SIMON G. KAPLAN, NIST — Our first-principles calculations and measurements of the far-infrared absorption in GaAs and GaP are presented and compared. Detailed frequency and temperature dependence are reported. Below the reststrahlen feature, a strong enhancement of the absorption is exhibited as the material is heated from 10 K to 300 K. The appearance of a phonon "gap" between acoustic and optical branches in GaP arises from the large ionic mass mismatch in that material, and causes a narrow infrared transmission band above the reststrahlen. Possible sources of discrepancy between experimental and theoretical spectra are addressed. These include the coexistence of two-phonon infrared channels independent of the anharmonic hybridization of two-phonon states with the infrared-active phonon, which is included in the calculation. Additional oscillator strength may be accounted for by considering direct two-phonon dipoles, or the higher-order charges. These additional channels account for the weak infrared absorption in diamond-type materials.

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