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Linear optical response of bulk GaAs from finite-temperature lattice dynamics A. SHKREBTII, University of Ontario Institute of Technology (UOIT), Oshawa, Canada, M.J.G. LEE, K. VYNCK, University of Toronto, Canada, T. TEATRO, D. ZEKVELD, UOIT, Oshawa, Canada, W. RICHTER, T. ZETTLER, T. TREPK, Technical University of Berlin, Germany — Measurements of the linear optical response of semiconductors are frequently carried out at and above room temperature, and linear optical probes are widely used to monitor various physical properties up to the melting point. We have found that Lorentzian broadening of the linear dielectric function, commonly used to model the effects of lattice vibrations, does not accurately describe the temperature dependence of the linear optical response. Instead, we determine the temperature dependence of the linear optical response of bulk GaAs in the temperature range 100 K to 1100 K from representative structural configurations extracted from finite-temperature molecular dynamics for an 8-atom supercell. The dielectric function corresponding to each structural configuration is calculated within the density functional theory (DFT) by the full-potential linearized augmented plane wave (FP-LAPW) method. The finite-temperature dielectric function is deduced by averaging the dielectric functions that correspond to the various structural configurations (about five structural configurations are sufficient for satisfactory convergence). The resulting finite-temperature dielectric functions are in good agreement with the experimental data over the whole temperature range.

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