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Modeling the optical dielectric function of semiconductors: Extension of the critical-point parabolic-band approximation

Charles C. Kim, J. W. Garland, H. Abad, and P. M. Raccah
Department of Physics, University of Illinois at Chicago, P.O. Box 4348, Chicago, Illinois 60680

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A model is proposed for the line shape of the optical dielectric function of zinc-blende semiconductors. For comparison with previously proposed models, this model is used primarily with spectroscopic ellipsometry data (but also transmission data below 1.5 eV) to obtain an analytic room-temperature dielectric function for GaAs. It is found to be more generally valid than the harmonic-oscillator model, the critical-point (CP) model, or the model of Adachi. It is applicable over the entire range of photon energies, below and above the lowest band gaps, incorporates the electronic band structure of the medium, and exactly satisfies the Kramers-Kronig transformation. It goes beyond the CP parabolic-band approximation in that it correctly takes into account the full analytic form of the electronic density of states and thus does not require the use of arbitrary cutoff energies. Also, it allows one to go beyond the usual approximation of Lorentzian broadening, which is known to be incorrect for elements and compounds above very low temperatures. For these reasons, it results in excellent quantitative agreement with experimental results for the dielectric function and for its derivatives with respect to photon energy, much better than that given by earlier models. Finally, the parameters of the model are physically significant and are easily determined as functions of composition for semiconductor alloys. Application of the model to the fitting of spectroscopic data on GaAs strongly suggests that spectroscopic ellipsometry does not measure the true bulk dielectric function. It also supports the conclusion that the line-shape broadening in GaAs at room temperature is more nearly Gaussian than Lorentzian.

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