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Modeling the Optical Constants of Diamond- and Zincblende-Type Semiconductors: Discrete and Continuum Exciton Effects at E_0 and E_1

1. F. H. Pollak,
2. M. Muñoz†,
3. T. Holden,
4. K. Wei,
5. V. M. Asnin

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Author Information

Physics Department and NY State Center for Advanced Technology in Ultrafast Photonic Materials and Applications, Brooklyn College of CUNY, Brooklyn, NY 11210, USA

†

Departamento de Fisica, CINVESTAV, Mexico DF, Mexico
Show messages
Email: F. H. Pollak (FHPBC@CUNYVM.CUNY.EDU), M. Muñoz (MARTIN@FIS.CINVESTAV.MX)

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Abstract

We present a comprehensive model dielectric function $\varepsilon(E)$ [$= \varepsilon_1 + i\varepsilon_2$] for diamond- and zincblende-type semiconductors based on the energy-band structure near critical points (CPs) plus discrete as well as continuum excitonic effects at the E_0, $E_0 + \Delta_0$, E_1, and $E_1 + \Delta_1$ CPs. In addition to the energies of these band-to-band CPs, our analysis also yields information about the binding energies of not only the 3D exciton associated with E_0 (R_0), when resolved, but also the 2D exciton related to the E_1, $E_1 + \Delta_1$ CPs (R_1). This model has been applied to spectral ellipsometry measurements of ε_1, ε_2 (0.3 eV < E < 5.5 eV) of ZnCdSe/InP, $CdTe_{1-x}S_x$, $In_{0.66}Ga_{0.34}As$, and GaSb and a surface photovoltage spectroscopy determination of the absorption coefficient of GaAs near E_0. This work shows conclusively that even if the exciton at E_0 is not resolved the lineshape is continuum exciton. The obtained values of R_1 exhibit a trend which is in good agreement with effective mass/$\mathbf{k} \cdot \mathbf{p}$ theory. Our analysis will be compared with the modeling of Adachi and the University of Illinois-Chicago group, both of whom neglect exciton continuum effects and hence have not evaluated R_1. Our results, particularly for exciton continuum effects at E_1, have considerable implications for recent first-principles band structure calculations which include exciton effects.

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