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Modeling the optical constants of CuGaSe2 and CuInSe2

Abstract.

The dielectric function data for CuGaSe₂ and CuInSe₂ have been modeled for both perpendicular ($E \perp c$) and parallel ($E \parallel c$) polarizations. We employ the modified Adachi's model dielectric function model with variable broadening. Variable broadening is accomplished by replacing the damping constant Γ with the energy-dependent expression $\Gamma(E)$, where the shape of the broadening function is determined by two adjustable model parameters. In spite of one additional parameter per transition, this model requires fewer parameters than the conventional Adachi s model to achieve equal or better agreement with the experimental data. Our calculations give the relative rms errors for the real and imaginary parts of the index of refraction, δ_n and δ_k , equal to 0.9% and 9.5% for CuGaSe₂ ($E \perp c$), 0.8% and 7.3% for CuGaSe₂ ($E \parallel c$), 1.1% and 3.0% for CuInSe₂ ($E \perp c$), and 2.5% and 3.7% for CuInSe₂ ($E \parallel c$), respectively.

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