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Modeling $\text{Al}_x\text{Ga}_{1-x}\text{As}$ optical constants as functions of composition

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Three models for the dielectric function $\epsilon_x(h\nu)$ of $\text{Al}_x\text{Ga}_{1-x}\text{As}$ are reviewed. All are based on measured optical constants at discrete compositions. The validity of each model near critical point energies, and otherwise, is evaluated. Only the energy-shift model is appropriate over the entire available spectrum (1.5–6.0 eV), including the band-gap (E_0) region.

This communication addresses the modeling of $\text{Al}_x\text{Ga}_{1-x}\text{As}$ optical constants as a function of composition x . Three different modeling approaches are described and compared. Applications include fitting spectroscopic data for heterostructure samples, e.g., in waveguide design, ellipsometric characterization, and more.

Aspnes *et al.* have measured the dielectric function $\epsilon(h\nu)$ in the range 1.5–6.0 eV for discrete nominal compositions $x = 0.0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7,$ and 0.8 .¹ The authors noted that compositional variation can be obtained by taking the weighted average of the two spectra closest in composition after their energy scales have been shifted to bring the nearest critical point energies into coincidence. It was suggested that this would only apply to a limited spectral range around the critical point energy E_1 .

We extended this approach to obtain $\epsilon(h\nu)$ over the entire measured spectrum, with continuous compositional variability.² With reference to Fig. 1 (from Ref. 1), three separate critical point regions are considered: E_0 , 1.4–2.5 eV; E_1 (and $E_1 + \Delta_1$), 2.9–3.9 eV; and E_2 , 4.8 eV. The energy positions of these critical points are given in Ref. 1 as

$$E_0(x) = 1.424 + 1.594x + x(1-x)(0.127 - 1.310x) \text{ eV}, \quad (1)$$

$$E_1(x) = 2.924 + 0.965x + x(1-x)(-0.157 - 0.935x) \text{ eV} \quad (2)$$

(E_2 is approximately independent of x).

For arbitrary x ($0.01 < x < 0.8$), we construct $\epsilon_x(h\nu)$ from $\epsilon_A(h\nu)$ and $\epsilon_B(h\nu)$, which are the measured dielectric functions with compositions $x_A < x < x_B$. Thus if $x = 0.37$, then $x_A = 0.3$ and $x_B = 0.4$ (more precise estimates of the actual compositions of the measured samples are given in Ref. 1; nominal values are used here). The construction consists of shifting the ϵ_A spectrum to higher energy, and the ϵ_B spectrum to lower energy, so that the critical point features coincide at an energy interpolated between the critical point energies of ϵ_A and ϵ_B , as described below. A weighted average of the two shifted spectra is then taken. This averaging accounts, to first order, for the small variation in amplitude with x (see Fig. 1).

The required energy shift for a given x is a function of

photon energy $h\nu$. At each of the two x -dependent critical point energies, the shifts are given by

$$\delta_{A,B}^{(E_0)} = |E_0(x) - E_0(x_{A,B})|, \quad (3)$$

$$\delta_{A,B}^{(E_1)} = |E_1(x) - E_1(x_{A,B})|. \quad (4)$$

The energies on the right-hand sides of (3) and (4) are given by (1) and (2). For photon energies other than E_0 and E_1 , the following piecewise linear interpolation is used. Below E_0 , $\delta(h\nu)$ is constant and equal to $\delta(E_0)$. Above E_2 , $\delta(h\nu)$ is zero. Between E_0 and E_1 , $\delta(h\nu)$ varies linearly between $\delta(E_0)$ and $\delta(E_1)$, and between E_1 and E_2 it varies linearly between $\delta(E_1)$ and zero. Figure 2 summarizes the energy shifts as functions of photon energy.

At a given photon energy, then, the calculated spectrum for x is the weighted average of the two shifted spectra:

$$\epsilon_x(h\nu) = \{\epsilon_A[h\nu - \delta_A(h\nu)](x_B - x) + \epsilon_B[h\nu + \delta_B(h\nu)](x - x_A)\} / (x_B - x_A). \quad (5)$$

The accuracy of ϵ_x computed in this algorithm depends on the accuracy of the original ϵ measurements, and the difference between x and the nearest endpoint, x_A or x_B .

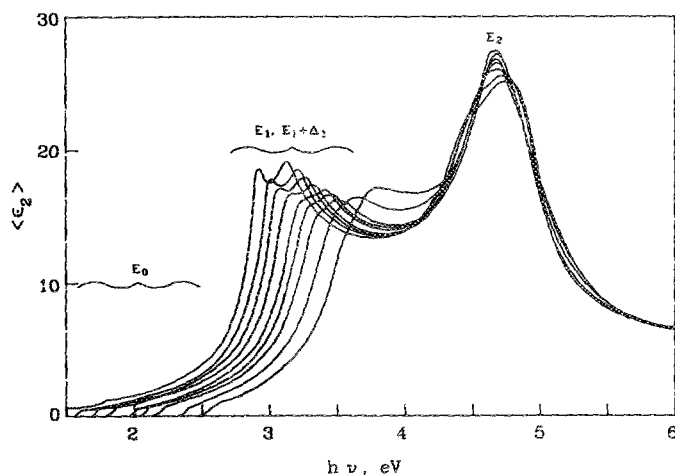


FIG. 1. Imaginary part of the dielectric function measured for $\text{Al}_x\text{Ga}_{1-x}\text{As}$, with x increasing from 0 in steps of approximately 0.1 (from Ref. 1).

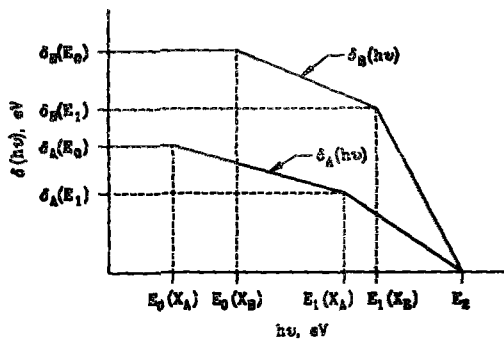


FIG. 2. Energy shifts $\epsilon(x_A)$ and $\epsilon(x_B)$, required to produce $\epsilon(x)$, are not constant over the spectrum. This is a simple scheme for smoothly varying the energy shifts, based on the known critical point energies $E_0(x)$ and $E_1(x)$.

The measured ϵ were estimated to be accurate to within 2% of the maximum value for $x < 0.5$, and to within 5% for $x > 0.6$.¹ For x coinciding with x_A or x_B , the weighting factor in Eq. (5) causes the calculated ϵ and its accuracy to be the same as the measured ϵ . For x midway between x_A and x_B , the accuracy is slightly degraded due to the piecewise linear approximation chosen for $\delta_{A,B}(h\nu)$.

A second approach is to use several discrete harmonic oscillators (HO) to model $\epsilon_x(h\nu)$. For each HO, the amplitude, center photon energy, and broadening parameter can be given as continuous functions of x , allowing $\epsilon(h\nu)$ to be calculated for any x . This physically appealing and relatively simple approach was used by Erman *et al.* to model GaAs with seven oscillators.³ The result is an accurate approximation to the measured ϵ over most of the spectrum. Unfortunately, the sharp onset of absorption at the band gap is not easily modeled with discrete oscillators, so no attempt was made to model the E_0 structure by including an oscillator at E_0 . Thus the HO model is only accurate at energies above, but not including, the E_0 region.

A third approach which has been taken is to use the Bruggeman effective-medium approximation (EMA) with two constituents, ϵ_A and ϵ_B .⁴ This model is not physically realistic for the case of $\text{Al}_x\text{Ga}_{1-x}\text{As}$, however. The EMA assumes a microscopic, but not atomic, mixture of the two constituents. Each "grain" is assumed to be large enough ($> 20 \text{ \AA}$) to retain its own characteristic bulk dielectric function, but much smaller than an optical wavelength. The EMA averages the two spectra, taking into account the electrical polarization that occurs at the grain boundaries, assuming approximately spherical grains.⁵

In the AlGaAs alloy, there are no grains, and thus no microstructural polarizing field to account for. Furthermore, since the EMA is an average of two spectra which are not energy shifted, critical point features from both spectra

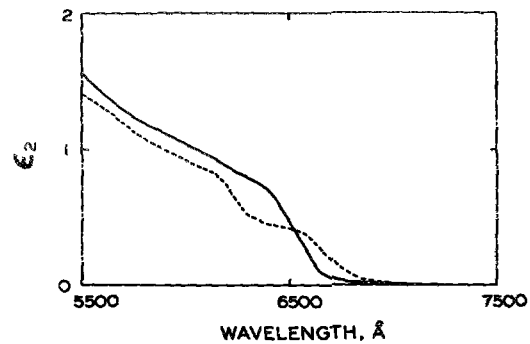


FIG. 3. ϵ_2 for $\text{Al}_{0.35}\text{Ga}_{0.65}\text{As}$ calculated from the measured $x = 0.3$ and $x = 0.4$ spectra, using the energy-shift model (solid) and the EMA model (dashed).

will appear in an EMA composite spectrum. This will be particularly evident at E_0 .

Figure 3 shows simulated $\epsilon_2(h\nu)$ near E_0 , for $x = 0.35$, using the energy-shift and the EMA models. The HO model would simply show a smoothly decaying ϵ_2 with increasing wavelength, and no structure at E_0 . The EMA spectrum contains *two* absorption edges, one from each constituent ($x_A = 0.3$ and $x_B = 0.4$), but no structure at $E_0(x = 0.35)$. The energy-shift model shows a single absorption edge at the appropriate band-gap energy.

It must be emphasized that the E_0 region is the most important region for waveguide applications. In addition, sensitivity to x is highest at E_0 , making it the most important region for characterization of composition. Optical constants in this region are *not* adequately modeled by the HO or EMA models.

Our previous work with GaAs/AlGaAs heterostructures clearly showed that ellipsometric data measured near E_0 are very sensitive to layer thicknesses and compositions.² The energy-shift model is most appropriate for this region, and it also works well over the rest of the spectrum. Other work⁶ has emphasized the E_1 region, where the HO model is also valid.

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