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Calculations of the Temperature and Alloy Composition Effects on the Optical Properties of $\text{Al}_x \text{Ga}_{1-x} \text{As}_y \text{Sb}_{1-y}$ and $\text{Ga}_x \text{In}_{1-x} \text{As}_y \text{Sb}_{1-y}$ in the Spectral Range 0.5-6 eV

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Calculations of the temperature and alloy composition effects on the optical properties of $\text{Al}_x\text{Ga}_{1-x}\text{As}_y\text{Sb}_{1-y}$ and $\text{Ga}_x\text{In}_{1-x}\text{As}_y\text{Sb}_{1-y}$ in the spectral range 0.5–6 eV

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A detailed analysis is presented on the temperature and alloy composition dependence of the optical properties of III-V alloys $\text{Al}_x\text{Ga}_{1-x}\text{As}_y\text{Sb}_{1-y}$ and $\text{Ga}_x\text{In}_{1-x}\text{As}_y\text{Sb}_{1-y}$ in the energy range 0.5–6 eV. Expressions for the complex dielectric function are based on a semiempirical phenomenological model, which takes under consideration indirect and direct transitions below and above the fundamental absorption edge. Dielectric function and absorption coefficient calculations are in satisfactory agreement with available experimental data. Other dielectric related optical data, such as the refractive index, extinction, and reflection coefficients, can also be obtained from the model.


I. INTRODUCTION

$\text{AlGaAsSb}$ and $\text{InGaAsSb}$ are semiconductor materials of increasing technological importance to optoelectronic devices. A detailed knowledge of their optical properties is essential for the design and fabrication of heterojunction photodetectors, thermophotovoltaic cells, infrared light-emitting diodes, fiber optics, and injection lasers.\textsuperscript{1–3}

The optical response of a material in terms of the incident radiation frequency ($\nu$) is fully described by the complex dielectric function $\varepsilon(\nu) = \varepsilon_r(\nu) + i\varepsilon_i(\nu)$, where the real and imaginary parts are related by the Kramers-Kronig transformation.\textsuperscript{4} The dielectric function is experimentally determined using various techniques, such as spectroscopic ellipsometry, reflectance measurements, and electron-energy-loss spectroscopy.\textsuperscript{1} Unfortunately, experimental measurements are not expressed as continuous analytic functions of the photon energy of the incident radiation. Modeling of the experimental dielectric function in terms of photon energy thus becomes crucial in the quantitative interpretation of the measured optical response, which helps in improving optoelectronic device design.

Several methods have been proposed in the literature for modeling the dielectric function. Depending on the approach taken, the different models can be classified as quantum mechanical or semiempirical in nature. Strict quantum-mechanical models utilize \textit{ab initio} or first-principle calculations to obtain both the real and imaginary parts of the dielectric function, considering the electron-hole pair interactions, i.e., the excitonic effects. Semi-quantum-mechanical models use first-principle calculations for the imaginary part of the dielectric function. Then, the Kramers-Kronig transformation is used to get the real part of the dielectric function from the imaginary part.\textsuperscript{4}

Semiempirical approaches for calculating the dielectric function include the damped harmonic oscillator model (DHO),\textsuperscript{4} the standard critical points model (SCP),\textsuperscript{5} the models by Fourouhi and Bloomer,\textsuperscript{6} Adachi,\textsuperscript{7–10} Holden \textit{et al.},\textsuperscript{11} and Kim and Sivananthan.\textsuperscript{12}

The DHO model describes the dielectric function in a phenomenological manner with the finite sum of Lorentz oscillators,\textsuperscript{4}

$$
\varepsilon(\nu) = 1 - \sum_{j=1}^{N} A_j \left( \frac{1}{h\nu + h\nu_j + i\Gamma_j} - \frac{1}{h\nu - h\nu_j + i\Gamma_j} \right),
$$

where $h$ is Planck’s constant, $h\nu$ is the photon energy of the incident radiation, $\Gamma_j$ is the adjustable damping constant (a phenomenological linewidth), $A_j$ is the fitted strength parameter, and $h\nu_j$ is the oscillator energy. The fitting improves with an increase in the number of oscillators, which in turn increases the number of adjustable parameters needed. The DHO model is not appropriate for describing the derivatives of the dielectric function, which allow a better determination of the critical points (CP) of the energy levels. Moreover, it has low accuracy below the fundamental band gap ($E_0$).\textsuperscript{1}

Also, parameters are generally not related to the band structure.

The SCP model takes into account the contributions from each critical point with analytical line shapes.\textsuperscript{5}
\[
e(\nu) = \sum_{j=1}^{N} \left[ C_j - A_j \exp(i\phi_j(h\nu - h\nu_j + i\Gamma_j)) \right],
\]

where the CP is described by an amplitude \( A_j \), nonresonant contribution \( C_j \), lifetime broadening (or damping constant) \( \Gamma_j \), CP energy threshold \( h\nu_j \), and excitonic phase angle \( \phi_j \). \( h\nu \) and \( \Gamma_j \) have similar meanings as in Eq. (1), but in this case correspond to a particular CP instead of an oscillator. The exponent \( n \) is equal to \(-\frac{1}{2}\) for one-dimensional (1D) CPs, \( n=0 \) [logarithmic, i.e., \( \ln(h\nu - h\nu_j + i\Gamma) \)] for two-dimensional (2D) CPs, \( n=\frac{1}{2} \) for three-dimensional (3D) CPs, and \( n=-1 \) for discrete excitons with Lorentzian line shape.\(^5\) The SCP model fits well to the derivatives of the dielectric function, but only moderately to the dielectric function itself.\(^1\)

The model of Forouhi and Bloomer\(^6\) is based on the quantum-mechanical theory of absorption. While the model has simple equations with a low number of parameters, only one parameter from the electronic band gap, \( E_0 \), is considered. The model is not appropriate for describing the derivatives of the dielectric function, and has low accuracy below \( E_0 \).\(^1\)

The dielectric function model proposed by Adachi\(^7\)–\(^10\) combines both the SCP model for the lowest energy levels and the DHO model for higher photon energy with undefined CPs [Eqs. (1) and (2)]. Contributions from indirect transitions and discrete and continuum excitons can be considered if needed, depending on the material. Adachi’s model is relatively simple, since all expressions are analytical in nature. Unfortunately, it is not very accurate around \( E_0 \). It also presents overestimation of the exciton related model parameters because the parameters for bound and unbound states are not independent.

Other models include those by Holden et al.,\(^11\) and Kim et al.\(^12\) The model of Holden et al. considers excitons plus band-to-band Coulomb enhanced line shapes near CPs, i.e., the Coulomb interaction between electron and hole. For higher energies, a DHO approximation is used. It expresses the dielectric function analytically and has a small number of parameters. This model is applicable for determining the Rydberg energies for 2D and 3D excitons, but has a number of intrinsic equations and leads to singularity when \( E=0 \).\(^1\) An extended absorption tail is produced in \( \varepsilon_2 \) due to the purely Lorentzian broadening, which has been artificially avoided (as in Adachi’s model) using a linear cutoff. To better fit experimental data, Kim et al. have considered Gaussian broadening in their model, approximated with a frequency-dependent analytical expression. This model fits well to the dielectric function and its derivatives, but has many intrinsic equations that are not analytical and require a large number of parameters. The frequency-dependent expression for \( \Gamma \) used by Kim et al. was later introduced into different models.\(^1,13\)–\(^15\)

Results from the quantum-mechanical approach show several discrepancies between the calculations and experimental data.\(^1\) The magnitude, sharpness, and position of the peaks do not necessarily coincide, and there are typically more structures in the computed curves than measured. We thus utilize a semiempirical phenomenological model akin to Adachi’s.\(^7\)–\(^10\) Since our main goal is to obtain the optical properties of AlGaAsSb and GaInAsSb as a function of both composition and temperature over a wide spectral range, more complicated models that introduce too many phenomenological parameters or are not fully expressed analytically are ill suited from a practical standpoint.

This article is organized as follows: Sec. II provides the theoretical model for calculating the dielectric function (Sec. II A), the temperature effects (Sec. II B), compositional dependencies (Sec. II C), and dielectric related optical constants (Sec. II D). In Sec. III, analysis and discussion of the calculated optical properties for both Al\(_{1-x}\)Ga\(_x\)As\(_{1-y}\)Sb\(_y\) (Sec. III A) and Ga\(_x\)In\(_{1-x}\)As\(_y\)Sb\(_{1-y}\) (Sec. III B) are given. Finally, conclusions obtained from this work are summarized in Sec. IV.

II. THEORETICAL MODEL

In order to model the optical properties of the quaternary materials under study, the dielectric function is calculated from semiempirical expressions for lower-lying transitions at major critical points in the joint density of states, and oscillators for higher-lying transitions. The final equation for the dielectric function over the spectral region 0.5–6 eV is expressed in terms of critical point energies and unknown parameters (e.g., strengths and lifetime broadenings) which are, to varying degrees, dependent upon composition and temperature. Thus, by carefully considering the variability of these parameters and the inherent relation of the optical constants to the dielectric function, it is possible to model the thermal and alloy composition effects on the optical properties of GaInAsSb and AlGaAsSb, the details of which are given in the following subsections.

A. Dielectric function calculation

The dielectric function of III-V semiconductors with a zinc-blende-type structure is dependent upon various transitions in energy levels deep in the valence band. In this work, we have considered transitions in the direct gap \( (E_0) \), spin-orbit split component \( (E_0 + \Delta_0) \), spin-orbit split doublet \( (E_1, E_1+\Delta_1) \), higher-lying \( E_2 \) peak, and indirect gap \( E_{ID}^0 \) \( (E_X \) or \( E_E \) \), which were found to offer the most significant contributions. Figure 1 illustrates the various transitions being considered for the case of the energy band structure of the Al\(_{1-x}\)Ga\(_x\)As\(_{1-y}\)Sb ternary compound in the AISb-rich composition domain.\(^16\)

We next discuss the various transitions involved. The contribution of the \( E_0(\Gamma) \) and \( [E_0(\Gamma) + \Delta_0(\Gamma)] \) energy gap involve transitions from 3D \( M_0 \)-type critical points and take place at the center point \( \Gamma \) of the Brillouin zone. Assuming parabolic bands, their contributions to the dielectric function are given by\(^4\)–\(^10\)

\[
e'(\nu) = AE_0^{-1.5} \left[ f\left(\frac{h\nu + i\Gamma}{E_0}\right) \right] + \frac{1}{2} \left( \frac{E_0}{E_0 + \Delta_0} \right)^{1.5} f\left(\frac{h\nu + i\Gamma}{E_0 + \Delta_0}\right),
\]

where
FIG. 1. Electronic energy-band structure of AlGa1−xSb in the AlSb-rich domain along several lines of high-symmetry direction, highlighting the transitions considered in the model (After Ref. 16).

The transition from the \(E_2(X)\) gap corresponds to a well-defined critical point. Thus, it is characterized by a Lorentz-type damped harmonic oscillator,5,10

\[
e^{III}(\nu) = \frac{C E_g^2}{E_c^2 - (hv)^2 - i\hbar \nu \Gamma},
\]

where \(C\) is a nondimensional (i.e., constant) strength parameter.

The transition from the indirect band gap \(E_g^{ID}\) is expressed as a second-order process in the perturbation, giving10

\[
e^{IV}(\nu) = \frac{2D}{\pi} \left[ -\left( \frac{E_g^{ID}}{E_c} \right)^2 \ln \left( \frac{h\nu + i\Gamma}{E_c} \right) + \frac{1}{2} \left( 1 + \frac{E_g^{ID}}{h\nu + i\Gamma} \right)^2 \ln \left( \frac{h\nu + i\Gamma + E_c}{h\nu + i\Gamma + E_g^{ID}} \right) + \frac{1}{2} \left( 1 - \frac{E_g^{ID}}{h\nu + i\Gamma} \right)^2 \ln \left( \frac{h\nu + i\Gamma - E_c}{h\nu + i\Gamma - E_g^{ID}} \right) \right].
\]

Here, \(D\) is the indirect gap strength parameter independent of the photon energy, and \(E_c\) is a high-energy cutoff, assumed equal to \(E_1\), which prevents nonphysical parabolic bands extending to infinite energies.

Finally, adding all individual contributions, from Eqs. (3), (5), (8), and (9), gives the complex dielectric function,

\[
e(\nu) = e'(\nu) + e''(\nu) + e^{III}(\nu) + e^{IV}(\nu).
\]

The Levenberg-Marquardt algorithm18,19 was used to fit all unknown model parameters through minimization of the cost function \(\chi^2\) (least-squares-fitting procedure) over all available experimental data points \(N\) at different temperatures and alloy composition,

\[
\chi^2 = \frac{1}{2} \sum_{i=1}^{N} \left[ (e_i^{\text{calc}}(\nu_i) - e_i^{\text{exp}}(\nu_i))^2 + [e_2(\nu_i)^{\text{calc}} - e_2^{\text{exp}}(\nu_i)]^2 \right],
\]

where the superscripts calc and exp stand for calculated and experimental dielectric function values, both corresponding to a particular \(i\)th photon energy.

Experimental dielectric function data at 300 K were obtained from Refs. 20 and 21 for GaAs, GaSb, InAs, and InSb; Ref. 22 for AlAs; Ref. 23 for AlSb; Ref. 24 for AlxGa1−xAs, Ref. 25 for InxGa1−xAs, and Ref. 26 for GaInxAsSb1−x. Dielectric data for various temperatures were taken from Refs. 27–31 for AlAs, InSb, GaAs, GaSb, and AlxGa1−xAs.

Table I provides fitted parameters used in the calculation of the dielectric function for each binary compound. From the simulations conducted, these parameters were found to have a negligible effect on the temperature variation of the dielectric constant, and thus have been assumed to remain constant. Remaining dielectric function parameters with greater temperature dependency, such as critical point energies and lifetime broadenings, are detailed in the following section.
B. Temperature effects

The dielectric function is strongly connected with the electronic energy band structures of the material. The variation of the critical point energy levels due to lattice thermal expansion and cation-phonon interactions (Debye-Waller effect) is described by the semi-empirical Varshni equation:32

\[
E(T) = E(T = 0) - \frac{\delta T^2}{(T + \beta)},
\]

where \(E(T=0)\) is the energy value extrapolated to absolute zero temperature; \(\delta\) and \(\beta\) are fitting constants. Table II shows the parameters used in Varshni’s equation.

Critical point peaks in dielectric function versus photon energy curves exhibit both a vertical and sideways shift with temperature variation.27–31 Substituting Eq. (12) in the dielectric function expressions given above [Eqs. (3) and (10)] mostly accounts for the horizontal displacement of the criti-

#### Table I. Basic fitted parameters used in the calculation of the dielectric function of each binary compound.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>AIAs</th>
<th>AISb</th>
<th>InAs</th>
<th>InSb</th>
<th>GaAs</th>
<th>GaSb</th>
</tr>
</thead>
<tbody>
<tr>
<td>(A[E_0(\Gamma)/E_0(\Gamma) + \Delta_e(\Gamma)]) (eV(1/3))</td>
<td>23.740</td>
<td>36.580</td>
<td>19.950</td>
<td>16.830</td>
<td>5.520</td>
<td>1.102</td>
</tr>
<tr>
<td>(C[E_0(X)])</td>
<td>2.240</td>
<td>1.600</td>
<td>1.750</td>
<td>2.640</td>
<td>2.890</td>
<td>3.340</td>
</tr>
<tr>
<td>(D[E_0^{1/2}]/)</td>
<td>0.705</td>
<td>1.190</td>
<td>21.511</td>
<td>38.830</td>
<td>21.320</td>
<td>4.93</td>
</tr>
<tr>
<td>(\Gamma[E_0(\Gamma)/E_0(\Gamma) + \Delta_e(\Gamma)]) (eV)</td>
<td>0.001</td>
<td>0.001</td>
<td>8.660</td>
<td>4.200</td>
<td>0.001</td>
<td>0.001</td>
</tr>
<tr>
<td>(\Gamma[E_0^{1/2}]/)</td>
<td>0.490</td>
<td>1.940</td>
<td>0.350</td>
<td>0.560</td>
<td>0.037</td>
<td>0.020</td>
</tr>
</tbody>
</table>

#### Table II. Parameters used in Varshni’s expression [Eq. (12)] to calculate the temperature dependence of the critical-point energies of each binary.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>AIAs</th>
<th>AISb</th>
<th>InAs</th>
<th>InSb</th>
<th>GaAs</th>
<th>GaSb</th>
</tr>
</thead>
<tbody>
<tr>
<td>Critical point energies</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(E_0(\Gamma))</td>
<td>3.09</td>
<td>0.88</td>
<td>530</td>
<td>33</td>
<td>2.39</td>
<td>0.42</td>
</tr>
<tr>
<td>(E_0(\Gamma) + \Delta_e(\Gamma))</td>
<td>3.37</td>
<td>0.88(^a)</td>
<td>530(^a)</td>
<td>33</td>
<td>3.06</td>
<td>0.42(^a)</td>
</tr>
<tr>
<td>(E_0(\Lambda))</td>
<td>3.98</td>
<td>0.67</td>
<td>0</td>
<td>27</td>
<td>2.94</td>
<td>0.47</td>
</tr>
<tr>
<td>(E_0(\Lambda) + \Delta_e(\Lambda))</td>
<td>4.18</td>
<td>0.67</td>
<td>0</td>
<td>27</td>
<td>3.43</td>
<td>0.43</td>
</tr>
<tr>
<td>(E_0(X))</td>
<td>4.86</td>
<td>0.32</td>
<td>0</td>
<td>27</td>
<td>4.18</td>
<td>0.47(^c)</td>
</tr>
<tr>
<td>(E_0^{1/2})</td>
<td>2.46(^b)</td>
<td>0.61</td>
<td>204</td>
<td>33</td>
<td>1.70(^d)</td>
<td>0.39</td>
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</table>

<table>
<thead>
<tr>
<th>Critical point energies</th>
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<tbody>
<tr>
<td>(E_0(\Gamma))</td>
<td>0.42</td>
<td>0.28</td>
<td>93</td>
<td>33</td>
<td>0.24</td>
<td>0.32</td>
</tr>
<tr>
<td>(E_0(\Gamma) + \Delta_e(\Gamma))</td>
<td>0.79</td>
<td>0.34(^a)</td>
<td>248(^a)</td>
<td>33</td>
<td>1.20</td>
<td>0.32(^a)</td>
</tr>
<tr>
<td>(E_0(\Lambda))</td>
<td>2.61</td>
<td>0.50</td>
<td>0</td>
<td>35</td>
<td>2.00</td>
<td>0.68</td>
</tr>
<tr>
<td>(E_0(\Lambda) + \Delta_e(\Lambda))</td>
<td>2.88</td>
<td>0.50(^c)</td>
<td>0(^c)</td>
<td>35</td>
<td>2.49</td>
<td>0.65</td>
</tr>
<tr>
<td>(E_0(X))</td>
<td>4.74</td>
<td>0.56</td>
<td>0</td>
<td>35</td>
<td>4.24</td>
<td>0.54</td>
</tr>
<tr>
<td>(E_0^{1/2})</td>
<td>1.13(^b)</td>
<td>0.28</td>
<td>93</td>
<td>33</td>
<td>0.93(^b)</td>
<td>0.32(^a)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Critical point energies</th>
<th></th>
<th></th>
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<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>(E_0(\Gamma))</td>
<td>1.52</td>
<td>0.55</td>
<td>225</td>
<td>29</td>
<td>0.81</td>
<td>0.42</td>
</tr>
<tr>
<td>(E_0(\Gamma) + \Delta_e(\Gamma))</td>
<td>1.85</td>
<td>0.35</td>
<td>225</td>
<td>29</td>
<td>1.57</td>
<td>0.42(^a)</td>
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<tr>
<td>(E_0(\Lambda))</td>
<td>3.04</td>
<td>0.72</td>
<td>205</td>
<td>29</td>
<td>2.19</td>
<td>0.68</td>
</tr>
<tr>
<td>(E_0(\Lambda) + \Delta_e(\Lambda))</td>
<td>3.27</td>
<td>0.72(^c)</td>
<td>205(^c)</td>
<td>29</td>
<td>2.62</td>
<td>0.67</td>
</tr>
<tr>
<td>(E_0(X))</td>
<td>5.13</td>
<td>0.66</td>
<td>43</td>
<td>29</td>
<td>4.32</td>
<td>0.90</td>
</tr>
<tr>
<td>(E_0^{1/2})</td>
<td>1.82(^b)</td>
<td>0.61</td>
<td>204</td>
<td>33</td>
<td>0.88(^b)</td>
<td>0.60</td>
</tr>
</tbody>
</table>

\(^a\)Temperature variance close to lowest direct gap shift, i.e., \(\Delta_e\) relatively constant.

\(^b\)Temperature variance assumed equal to \(E_1\) shift.

\(^c\)\(E_0(\Gamma)\)\(\rightarrow\)\(L_6\).

\(^d\)\(E_0(\Gamma)\)\(\rightarrow\)\(X_{6c}\).

\(^e\)\(E_0(\Gamma)\)\(\rightarrow\)\(L_6\).
is determined by a reduction of lifetime broadening of the pounds. Experimental dielectric-temperature data for these two compounds is assumed to be similar to the other binaries due to a lack of ternary compounds:21,22,24 Their temperature dependence was approximated with the following linear function:28

$$\Gamma(T) = \Gamma_L + \gamma T,$$  \hspace{1cm} (13)

where both $\Gamma_L$ and $\gamma$ are fitted constants. The first term represents the lifetime broadening caused by temperature-independent mechanisms.31 Fitted values for $\Gamma_L$ and $\gamma$ are listed in Table III. Considering dielectric function data at 300 K $\Gamma_{E_{2}(E_{1}+E_{A})}$ and $\Gamma_{E_{2}}$ were found to be 0.017 and 0.785 meV for AlSb and 0.0903 and 0.493 meV for InAs, respectively. Their temperature dependence was assumed to be similar to the other binaries due to a lack of experimental dielectric-temperature data for these two compounds.

The lattice constant $[a_{lc}$ in Eqs. (6) and (7)] expands linearly with increasing temperature, as given by the following expression:33

$$a_{lc}(T) = a_{lc}(300) + \kappa(T - 300),$$  \hspace{1cm} (14)

where the first term represents the lattice constant at 300 K and $\kappa$ is a temperature coefficient. Parameter values in Eq. (14) were taken from Ref. 33 and are listed in Table IV.

**C. Composition dependence**

The quaternary material $A_xB_{1-x}C_yD_{1-y}$ is constructed of four binary compounds: $AC$, $AD$, $BC$, and $BD$; or else of four ternary compounds: $A_xB_{1-x}C_y$, $A_xB_{1-x}D_y$, $AC_yD_{1-y}$, and $BC_yD_{1-y}$. In particular, for AlGaAsSb with form $A_xB_{1-x}C_yD_{1-y}$, its binary compounds are $AC=AlAs$, $AD=AlSb$, $BC=GaAs$, and $BD=GaSb$. Its ternary compounds are $ABC=AlGaAs$, $ABD=AlGaSb$, $ACD=AlAsSb$, and $BCD=GaAsSb$. Considering GaInAsSb with form $A_xB_{1-x}C_yD_{1-y}$, the binary compounds are $AC=GaAs$, $AD=GaSb$ and $BC=InAs$ and $BD=InSb$. The ternary compounds are $ABC=GaInAs$, $ABD=GaInSb$, $ACD=GaAsSb$, and $BCD=InAsSb$.

The material parameters for ternary semiconductors ($T$) in the form $A_xB_{1-x}C$ are commonly obtained from the linear interpolation of the transition parameters of the binary materials ($B$) using Vegard’s law,36,37

$$T_{ABC}(x) = xB_{AC} + (1-x)B_{BC} - x(1-x)C,$$  \hspace{1cm} (15)

where $C$ is a bowing constant that accounts for deviations from the linear interpolation due to lattice disorders arising from the presence of different cations. Once the ternary parameters are known via interpolation, the quaternary parameters ($Q$) for the lower energy levels (alloy in the form $A_xB_{1-x}C_yD_{1-y}$) are obtained using the method of Glisson et al.,38,39

$$Q_{ABCD}(x,y) = \frac{1}{x(1-x)+\gamma(x(1-x)\gamma T_{ABC}(x) + (1-x)T_{BCD}(y) + (1-y)\gamma T_{ACD}(y))},$$  \hspace{1cm} (16)

The quaternary material parameters (form $A_xB_{1-x}C_yD_{1-y}$) may also be obtained from the binary parameters using Vegard’s rule,36,39

$$Q_{ABCD}(x,y) = xyB_{AC} + x(1-y)B_{AD} + (1-x)yB_{BC} + (1-x)(1-y)B_{BD} + C_{A-B}x(1-x) + C_{C-D}(1-y).$$  \hspace{1cm} (17)

In the above expression, bowing parameters $C_{A-B}$ and $C_{C-D}$ are assumed to arise from independent anion-cation sublattice disorders. Since bowing constants for critical point energies of several ternary III-V semiconductors are available in the literature, we shall then calculate the quaternary energy transitions by making use of Eqs. (15) and (16). For all other model parameters, Eq. (17) is used, with both $C_{A-B}$ and $C_{C-D}$ fitted to experimental data.20–26 Temperature is assumed to have a negligible effect on bowing parameters, since, as of yet, there is no significant data analysis or analytic interpretation in this regard for several materials.33

Table V gives the bowing constants used in the calculation of the various critical point energy transitions for each ternary. Unknown bowing parameters for the indirect band gap are estimated as follows:39

$$C(E_g^D) = 1/2[C(E_0) + C(E_1)],$$  \hspace{1cm} (18)

where $C(E_0)$ and $C(E_1)$ are the bowing parameters for the $E_0$ and $E_1$ gaps.

For the spin split-off band, the following approximation is used:39

$$C(E_g^S) = 1/2[C(E_0) + C(E_1)].$$  \hspace{1cm} (19)
TABLE V. Bowing parameters (in eV) used in the linear interpolation of the critical-point energies for each ternary compound [Eq. (15)] of AlGaAsSb and InGaAsSb at 300 K.

<table>
<thead>
<tr>
<th>Ternary</th>
<th>C(E₀)</th>
<th>C(E₀ + Δ₀)</th>
<th>C(E₁)</th>
<th>C(E₁ + Δ₁)</th>
<th>C(E₀ - ID)</th>
<th>C(E₀ - ID)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al₀.₃Ga₀.₇Sb₀.₇</td>
<td>0.72⁴</td>
<td>0.15⁹</td>
<td>⋯</td>
<td>⋯</td>
<td>⋯</td>
<td>0.28¹</td>
</tr>
<tr>
<td>Ga₀.₇As₀.₃Sb₀.₇</td>
<td>1.2⁵</td>
<td>0.6¹</td>
<td>⋯</td>
<td>⋯</td>
<td>0.06⁴</td>
<td>0.1⁵</td>
</tr>
<tr>
<td>In₀.₃Sb₀.₇As₀.₃</td>
<td>0.6⁸</td>
<td>1.2²</td>
<td>0.5³</td>
<td>0.4⁷</td>
<td>0.6⁵</td>
<td>0.5⁷</td>
</tr>
<tr>
<td>Al₀.₃Ga₀.₇As₀.₇</td>
<td>0.3⁷</td>
<td>0.0⁷</td>
<td>0.4⁶</td>
<td>0.0²²</td>
<td>0.06⁶</td>
<td>0.0⁶²</td>
</tr>
<tr>
<td>Ga₀.₃In₀.₇As₀.₃</td>
<td>0.0⁷</td>
<td>0.0²²</td>
<td>0.5⁶</td>
<td>0.0²²</td>
<td>0.7²</td>
<td>0.7²²</td>
</tr>
<tr>
<td>Al₀.₃Ga₀.₇Sb₀.₇</td>
<td>0.6⁴³</td>
<td>0.1⁰</td>
<td>0.3⁸</td>
<td>0.2⁸</td>
<td>⋯</td>
<td>0.2⁴²</td>
</tr>
<tr>
<td>Ga₀.₃In₀.₇Sb₀.₇</td>
<td>0.4²</td>
<td>0.1⁰</td>
<td>0.3⁸</td>
<td>0.2⁸</td>
<td>⋯</td>
<td>0.2⁴²</td>
</tr>
</tbody>
</table>

References:
①Reference 43.
②Reference 44.
③Reference 45.
④Estimated in this study. See the text.
⑤Reference 46.
⑥Reference 47.
⑦Reference 48.
⑧Reference 49.
⑨Reference 50.
⑩Reference 14.
⑪Reference 51.
⑫Reference 32.

\[ C(\Delta_0) = (\Delta_{01}/E_1)C(E_0), \]

where \( \Delta_{01} \) and \( E_1 \) are the linearly interpolated values at \( x = 0.5 \) of \( \Delta_0 \) and \( E_0 \) from the limiting compounds. Table VI lists the bowing parameters fitted to Eq. (17) for both quaternaries.

### D. Optical coefficients

Once the dielectric function for a certain alloy composition and temperature is determined, the real part of the complex refractive index \( n \) and its imaginary part \( k \) (the extinction coefficient or attenuation index), can be calculated using the following expressions: \(^{21}\)

\[ n = \left( \frac{(\varepsilon_2^2 + \varepsilon_3^2)^{1/2} + \varepsilon_1}{2} \right)^{1/2}, \]

\[ k = \left( \frac{(\varepsilon_2^2 + \varepsilon_3^2)^{1/2} - \varepsilon_1}{2} \right)^{1/2}. \]

The normal incidence reflectivity \( R \) and the absorption coefficient \( \alpha \) are then expressed in terms of \( n \) and \( k \) as follows: \(^{21}\)

\[ R = \frac{n - ik - 1}{n - ik + 1} \left( \frac{n + 1}{n + 1 + k^2} \right)^{1/2}, \]

\[ \alpha = \frac{4\pi k}{\lambda}, \]

where \( \lambda \) is the wavelength of the incident radiation in vacuum.

### III. ANALYSIS AND DISCUSSION

Contributions to the dielectric constant arise from several partitions of the Brillouin zone. The percentiles of each contribution were estimated to be in accordance with those reported in Ref. 40. The \( L \) region with corresponding \( E_1 \) and \( E_2 \) transition energies contributes approximately 65–70% to the total value of the dielectric constant. The \( \Gamma \) region corresponding to the \( E_0 \) transition accounts for 5–10% of the total. The \( E_2 \) and \( E_2' \) transitions in the \( X \) region account for 15–30% of the total.

We have considered only the dominant indirect transitions, i.e., \( E_4(\Gamma_{SV} \rightarrow \Gamma_{AC}) \) for AlSb and \( E_4(\Gamma_{SV} \rightarrow L_{AC}) \) for all other binaries. Excitonic states in principle exist at each type of critical point, since Coulomb-type interactions are always present between electrons and holes. \(^{30}\) In fact, at very low temperatures, the excitonic effects profoundly modify the critical points singularity structure, making the one-electron approximation unsuitable. However, excitonic effects are not observed if the thermal energy exceeds the exciton binding energy or the screening effects push the exciton levels into the continuum of the conduction band. In particular, contributions to the dielectric function from 3D discrete excitonic effects near the \( E_0 \) critical point can be neglected because of the narrow spectral range of these transitions. \(^{10,40}\) Contributions from continuous excitations at the \( E_0 \) and higher transitions are very similar to noninteracting electron-hole pair characteristics. \(^{10}\) Thus, for temperatures of 150 K and above, excitonic effects are not as important and the one-electron approximation becomes suitable for most practical applications.

#### A. AlₓGa₁₋ₓAsₓSb₁₋ₓ

The \( Al_{x_{Ga_{1-x}}As_{y}Sb_{1-y}} \) quaternary alloy is characterized by a relatively large band gap that covers the wavelength range between the visible and infrared regions (0.57–1.72 \( \mu \)m). \(^{39}\) The alloys can be grown lattice matched to commercially available binary substrates, such as GaSb, InP, and InAs. However, miscibility gaps may limit the range of homogenous solid-phase alloy compositions. \(^{39}\) AlGaAsSb lattice matched to GaSb is a natural energy barrier to majority carrier transport and is typically used as a cladding layer of fluoride glass fibers and emitters of heterojunction phototransistors due to its lower refractive index. \(^{33,39}\)

The alloy systems \( Al_{x_{Ga_{1-x}}As_{y}Sb_{1-y}}/GaSb \) and \( Al_{x_{Ga_{1-x}}As_{y}Sb_{1-y}}/InAs \) present a transition between direct and indirect structures at approximately \( x \approx 0.45^{.39} \). The \( E_0 \) gap at the \( \Gamma \) point is very close to the \( E_2^D \) gap at the \( L \) point, causing an injected-electron loss and consequently a large threshold current. \(^{39}\) Sb-based systems have a relatively high
spin split-off gap $\Delta_0$ Auger recombination and intervalence-band optical transitions related to the $\Delta_0$ gap that play an important role in the device operation characteristics, i.e., threshold current and its temperature dependence.\textsuperscript{39} AlGaAsSb systems have a large refractive index step within the whole range of alloy composition.

The room-temperature complex dielectric function of the Al$_x$Ga$_{1-x}$As$_y$Sb$_{1-y}$ alloy is shown in Fig. 2 for six different compositions [real part $\varepsilon_1$, shown in Fig. 2(a) and imaginary part $\varepsilon_2$, shown in Fig. 2(b)]. The solid lines are numerically obtained from the model using Eqs. (3) and (10) to account for the various energy levels contribution, and Eqs. (15) and (17) to calculate the composition dependence of all parameters. Critical point energies are pointed out for the uppermost dielectric curve for Al$_{0.72}$Ga$_{0.28}$As$_{0.18}$Sb$_{0.82}$. The shift of the three dominant structures $E_1$, $E_1+\Delta_1$, and $E_2$ to higher energy with increasing Al composition $x$ is evident from looking at the figure. The $E_1$ and $E_1+\Delta_1$ peaks in the $\varepsilon_2$ spectrum are more resolved at the end points $x=0.00$ and $x=1.00$, while they lose their strengths at intermediate compositions approaching $x\sim0.5$. These broadening dependences are related to statistical fluctuations of the crystal potential in the alloy, which tend to dominate over potential contributions arising from bulk dislocations.\textsuperscript{25,37} Reasonable agreement between the modeled dielectric function curves and experimental data is obtained around the lower direct energy gaps $E_0$ and $E_0+\Delta_0$, indirect band $E_{\text{ID}}$, and the higher-lying $E_2$ CP. In the vicinity of the $E_1$ and $E_1+\Delta_1$ CPs, calculated curves present somewhat lower and more pronounced peaks than experimental data for both $\varepsilon_1$ and $\varepsilon_2$. Better agreement is obtained if fitted values are used for the strength parameters $B_1$ and $B_2$ in Eq. (5) instead of calculat-
shown in Fig. 2 to demonstrate the capabilities of the model.

which experimental data are not presently available, is also
ponents of the dielectric function of Al$_{0.27}$Ga$_{0.73}$As at tem-
function for one such quaternary, Al$_{0.72}$Ga$_{0.28}$As$_{0.18}$Sb$_{0.82}$, for
not been studied previously. A prediction of the dielectric
calculation of the optical properties of quaternaries that have
tradeoffs under consideration, the model offers a fairly accu-
such as oxides or air pollutants. Taking all these facts and
present "pseudodielectric" function data, as they were de-
exist in the experimental conditions under which the various
data considered were obtained. For example, Refs. 20 and 24

FIG. 3. Real ($\varepsilon_1$) and imaginary ($\varepsilon_2$) components of the dielectric function ($\varepsilon$) of Al$_{0.27}$Ga$_{0.73}$As at 300, 515, and 685 K. Calculated values (lines) correspond to experimental data in Ref. 31 (symbols). The arrows highlight the critical point energies at 300 K.

ing them with Eqs. (6) and (7). However, since these expres-
sions for $B_1$ and $B_2$ are functions of energy and lattice con-
stant, they allow for a better consideration of temperature effects in a more physical manner while still offering a rea-
sonably good agreement with experiments in light of the
 crudeness of the theory employed. Moreover, discrepancies
exist in the experimental conditions under which the various
data considered were obtained. For example, Refs. 20 and 24
present "pseudodielectric: function" data, as they were ded-
uced from reflectance of samples with surface contaminants
such as oxides or air pollutants. Taking all these facts and
tradeoffs under consideration, the model offers a fairly accu-
rate representation of the dielectric function for various com-
positions including the temperature effects, and enables the
calculation of the optical properties of quaternaries that have
not been studied previously. A prediction of the dielectric
function for one such quaternary, Al$_{0.72}$Ga$_{0.28}$As$_{0.18}$Sb$_{0.82}$, for
which experimental data are not presently available, is also
shown in Fig. 2 to demonstrate the capabilities of the model.

Figure 3 depicts the real part $\varepsilon_1$ and imaginary $\varepsilon_2$
ponents of the dielectric function of Al$_{0.27}$Ga$_{0.73}$As at tem-
peratures of 300, 515, and 685 K. Numerical data (lines) are
computed using Eqs. (12) and (14) to calculate the tempera-
ture dependence of CP energy levels, lifetime broadenings,
and lattice expansion, substituted into the dielectric function
Eqs. (3) and (10) for every energy level contributions, Com-
position values are fixed at $x=0.27$ and $y=1$ in Eqs. (15)
and (17). Both vertical and horizontal temperature shifts in the
CP peaks are clearly visible in Fig. 3. The change in the CP
energy levels with temperature, as described by Eq. (12),
causes the dielectric function to move sideways. The hori-
zontal shifts in the peaks are more pronounced around the
$E_1$, $E_1+\Delta_1$, and $E_2$ peaks, corresponding to significant tem-
perature variation in the CP lifetime broadenings around $\Lambda$
and $X$, approximated with Eq. (13). In the model, the $E_1$
and $E_1+\Delta_1$ peaks are also affected by the lattice constant, which
expands with increasing temperature. The model is not ap-
licable below 150 K, since the CP energies at very low
 temperatures are not well known for some of the binary con-
stituents. The energy temperature dependence of these mate-
rials was thus assumed linear, which is the case above 150
K. Moreover, the exact behavior of the energy bands
expands with increasing temperature. The model is not ap-

FIG. 4. Absorption coefficient $\alpha$ of Al$_{x}$Ga$_{1-x}$As$_{y}$Sb$_{1-y}$ at 300 K for various compositions. Experimental data are taken from Ref. 20 (+), Ref. 23 (+), Ref. 24 (×) (●), and Ref. 42 (∆).

J. Appl. Phys. 102, 014504 (2007)
taken from Refs. 20, 23, 24, and 42. Energy peaks are highlighted in the figure for the uppermost absorption data, corresponding to the GaSb binary.

**B. Ga\textsubscript{x}In\textsubscript{1-x}As\textsubscript{y}Sb\textsubscript{1-y}**

The Ga\textsubscript{x}In\textsubscript{1-x}As\textsubscript{y}Sb\textsubscript{1-y} alloys are suitable for devices operating in the 24 µm spectral region needed for low-loss fluoride glass fibers cores and phototransistor collectors. Like Al\textsubscript{x}Ga\textsubscript{1-x}As\textsubscript{y}Sb\textsubscript{1-y}, Ga\textsubscript{x}In\textsubscript{1-x}As\textsubscript{y}Sb\textsubscript{1-y} may be grown lattice matched on GaSb, InP, and InAs. GaInAsSb lattice matched to GaSb is an important active-region constituent of diode lasers emitting at \(\lambda=2\ \mu\text{m}.\)\textsuperscript{33} The cutoff wavelengths of GaInAsSb lattice matched to InP are close to the 1.55 µm low-loss window for optical fiber communications.

GaInAsSb/InP usefulness is limited, however, because both end points have nearly the same energy gap (0.71–0.86 eV).\textsuperscript{33,39} The band-gap energy varies in the range 0.3–0.71 and 0.36–0.69 eV when lattice matched to GaSb and InAs, respectively. Unlike Al\textsubscript{x}Ga\textsubscript{1-x}As\textsubscript{y}Sb\textsubscript{1-y}, the absorption at the fundamental optical gaps in Ga\textsubscript{x}In\textsubscript{1-x}As\textsubscript{y}Sb\textsubscript{1-y}/GaSb and Ga\textsubscript{x}In\textsubscript{1-x}As\textsubscript{y}Sb\textsubscript{1-y}/InAs is direct within the whole range of alloy composition.

The quaternary Ga\textsubscript{x}In\textsubscript{1-x}As\textsubscript{y}Sb\textsubscript{1-y} lattice matched to InAs and GaSb presents a refractive index anomaly in the sense that the material with smaller \(E_0\) gap has a lower refractive index, while the opposite behavior is common to most III-V alloys.\textsuperscript{39} This is mainly due to alloy disorder effects, i.e., intraband and interband interactions, which break
the symmetry of the crystal lattice in Sb-based compounds and cause the band structure constants related to the refractive index to present nonlinearity with alloy composition.\(^3\)

The real part \(\varepsilon_1\), shown in Fig. 5(a), and imaginary part \(\varepsilon_2\), shown in Fig. 5(b), of the complex dielectric function of Ga\(_{0.48}\)In\(_{0.52}\)As\(_2\) are calculated for six different compositions at room temperature. The solid lines represent dielectric function calculations using Eqs. (3) and (10) to account for energy gap transitions and Eqs. (15) and (17) to account for the composition dependence, as with Al\(_x\)Ga\(_{1-x}\)As\(_2\). Curves for each composition are offset by increments of 10 starting from GaAs. Critical point energies are indicated for the uppermost curves. For either Ga\(_x\)As or Ga\(_x\)Sb, CPs \(E_1\), \(E_1+\Delta_1\), and \(E_2\) shift to higher energy with increasing \(x\), as is the case for Al\(_x\)Ga\(_{1-x}\)As\(_2\). The \(E_1\) and \(E_1+\Delta_1\) peaks are sharper for \(x=0.00\) and \(x=1.00\) and weaker at intermediate compositions due to statistical fluctuations of the crystal potential.\(^{25,37}\) Better agreement with experiments is obtained around \(E_0, E_0+\Delta_0, E_0^{\beta},\) and \(E_2\), while the \(E_1\) and \(E_1+\Delta_1\) CPs have weaker but more pronounced peaks than experiments due to the inclusion of Eqs. (6) and (7) to calculate the \(B_1\) and \(B_2\) strength parameters, the justification of which has been given previously. The accuracy of the calculated results is expected to be similar to the Al\(_x\)Ga\(_{1-x}\)As\(_2\) case.

Experimental dielectric function data for the ternaries and quaternaries of Ga\(_{1-x}\)In\(_x\)As\(_2\) at temperatures other than 300 K are not readily available. We thus make a prediction based on the temperature behavior of the binaries and their interpolation. Figure 6 shows the real (\(\varepsilon_1\)) and imaginary (\(\varepsilon_2\)) components of the dielectric function of the widely studied ternary Ga\(_{0.48}\)In\(_{0.52}\)As\(_2\) at 150, 300, 515, and 685 K. Lines correspond to the values obtained from the model, while circles represent room-temperature experimental data taken from Ref. 25. The vertical shift in the peaks of the dielectric function to higher energy with decreasing temperature corresponds to the CP energies increase due to lattice thermal contraction with cooling and cation-phonon interactions, considered in Eq. (12). The horizontal increase in the \(E_1\), \(E_1+\Delta_1\), and \(E_2\) peaks with lower temperature is caused by the temperature shift in the CP lifetime broadening parameters with \(\Lambda\) and \(X\) [Eq. (13)].

Figure 7 shows the absorption coefficient of Ga\(_{1-x}\)In\(_x\)As\(_2\) at 300 K for various compositions. Lines correspond to values obtained from the model [Eq. (23)]. Selected absorption experimental data, represented in Fig. 7 by symbols, are taken from Refs. 20, 21, and 26. Critical point energies are marked for InSb. The shift in the cutoff photon energy \(E_0\) is lowest for InSb (\(x=0, y=0\)) and highest for GaAs (\(x=1, y=1\)), both binary end points.

IV. CONCLUSIONS

The complex dielectric function and related optical properties of AlGaAsSb and GaInAsSb are analyzed in the
photon-energy range 0.5–6 eV using a semiempirical phenomenological model. The effects of both alloy composition and temperature on the dielectric function are incorporated into the model considering a linear interpolation scheme as well as band gap, broadening, and lattice constant distortions. The methodology for calculation of various device parameters in the AlGaAsSb and GaInAsSb alloy systems is analyzed, and results are presented which could aid in the design of optoelectronic devices.

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