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Noise modeling for W-band pseudomorphic InGaAs HEMT’s
Modeling the optical dielectric function of GaAs and AlAs: Extension of Adachi’s model

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Optical dielectric function model of Ozaki and Adachi [J. Appl. Phys. 78, 3380 (1995)] is augmented by introducing Gaussian-like broadening function instead of Lorentzian broadening. In this way a consistent and comparatively simple analytic formula has been obtained, which accurately describes the optical dielectric function of GaAs and AlAs in a wide spectral range between 0.1 and 6 eV. The acceptance-probability-controlled simulated annealing technique was used to fit the model to experimental data. © 1996 American Institute of Physics.

I. INTRODUCTION

GaAs and AlAs are semiconductors of technological importance to both in-plane semiconductor lasers and vertical cavity lasers, photodetectors and other optoelectronic devices. The knowledge of their refractive indices and absorption coefficients over a wide range of optical wavelengths is essential in the design and analysis of distributed Bragg reflectors used in vertical cavity surface emitting lasers and vertical cavity modulators.

It is well known that the optical properties of solids can be described in terms of the complex optical dielectric function \( \varepsilon_r(\omega) = \varepsilon_{r1}(\omega) + i \varepsilon_{r2}(\omega) \). It is a significant shortcoming that the experimental \( \varepsilon_r(\omega) \) is not expressed as a function of critical point (CP) energies \( E_j \). This deficiency can be overcome by using models.

A semiempirical single effective oscillator model of Wemple and DiDomenico\(^5,6\) has been used to model the dispersion sufficiently below the direct band gap in more than 50 nonmetallic solids. Certainly, this model is not applicable in the \( E_0 \) critical point region and above. Aframowitz\(^3\) has proposed a model which takes into account the direct absorption edge (\( E_0 \)) and which yields a reasonably good agreement with experiment on the low-energy side of the spectrum. This simple model including its recent modifications\(^4,5\) have been frequently used for device design purposes.\(^6-11\)

Erman’s model,\(^12\) based on the damped harmonic oscillator (DHO) approximation, has been widely used to calculate the optical dielectric function versus frequency and alloy composition\(^12-15\) and to model the temperature dependence of the optical dielectric function\(^16-19\) at energies well above the first CP energy \( E_0 \). Most recently the same model has been used in modelling apparent optical dielectric function of strained films.\(^20\) Using a large number of oscillators DHO model yields accurate fit above the \( E_0 \). However, the DHO model is not applicable for describing the absorption \( [\varepsilon_{r2}(\omega)] \) in the \( E_0 \) CP region and below. Furthermore, due to the phenomenological character of the DHO model, the inclusion of temperature or alloy composition dependence is rather complicated.

The first model proposed by Adachi (1982) was a simplified interband transition model\(^21,22\) which includes \( E_0 \) and \( E_0 + \Delta_0 \) transitions to interpret optical dielectric function near and below the fundamental absorption edge. Although the dispersion in this region can be attributed to the two lowest-lying gaps (\( E_0 \) and \( E_0 + \Delta_0 \)), the absolute value of the \( \varepsilon_{r1}(\omega) \) is determined, mainly, by the higher-lying-gap transitions. In this model, the contribution from these transitions is described by an additive, frequency-independent term. Substantial improvement of the simplified interband transition model is a composite model by Adachi\(^23,24\) which augments the forementioned model by incorporating terms that describe \( E_1 \) and \( E_1 + \Delta_1 \) transitions and with phenomenological terms that describe contributions from higher-lying direct transitions. Adachi’s composite model\(^23,24\) was much acclaimed as a relatively simple, yet fairly accurate model for the optical dielectric function. Several extensions and modifications to this model have been published recently.\(^25-30\)

However, there is a problem inherent to all the models described hitherto. They do not adequately describe the absorption in the vicinity of the direct edge (the \( E_0 \) CP region) and below.

In a recent series of papers, Kim et al.\(^31-33\) have proposed an accurate but rather intricate model which includes, theoretically, both cases of Lorentzian and Gaussian broadening. Their model with the Gaussian broadening shows significantly better agreement with experiment in the vicinity of \( E_0 \) as compared to the model with the Lorentzian broadening. In the \( E_0 \) CP region, the behavior of Kim’s model with Lorentzian broadening is, in spite of its accurate functional representation for the joint density of states, very similar to that of the Adachi’s model. This suggests that it is not only the functional form of the joint density of states (or momentum matrix element) but also the type of the broadening-function approximation that is responsible for the large discrepancies between Adachi’s model\(^29\) and experiment in the \( E_0 \) region. In this article we show that by assuming the Gaussian-like broadening function, the accuracy of the recent model by Ozaki and Adachi\(^29\) can be significantly improved. It is further shown that with this improvement, our model can accurately describe both the absorption and dispersion in
GaAs and AlAs even in the $E_0$ CP region where the same model with Lorentzian broadening is highly inaccurate. The model described in this article gives comparatively a simple analytic formula which describes accurately the dielectric function of GaAs and AlAs in a wide spectral range between 0.1 and 6 eV. Hence, the absorption and dispersion below, at, and above the first critical point $E_0$ can be readily obtained. Furthermore, the model proposed in this paper can easily be modified to describe the alloy composition and temperature dependence of the optical dielectric functions of GaAs and AlAs. Fitting the model to data is performed using the acceptance probability controlled simulated annealing technique, a combinatorial optimization algorithm specifically designed for multiparameter fitting purposes.

This article is organized as follows. In Sec. II the effect of the broadening function on the imaginary part of the $\varepsilon_i(\omega)$ is described. In Sec. III a brief description of the proposed model is given. In Sec. IV the fitting algorithm is outlined and applied to determine the model parameters for GaAs and AlAs. Further, in Sec. IV the dielectric constants calculated using our model are compared with experimental data and other models.

II. THE EFFECT OF THE BROADENING FUNCTION

The interband absorption is accompanied by the lifetime broadening, a damping effect caused mainly by electron-phonon and electron-defect interaction. The optical dielectric function of a solid, with line broadening described by the damping function $\gamma(s)$ is given by

$$\varepsilon_i(\omega) = 1 + \frac{2\hbar^2 e^2}{\varepsilon_0 m^*} \sum_{c,v} \int E_{cv}(E) dE \left( \frac{P_{cv}(E)}{E} \right)^2 \times \left[ \int_0^\infty ds e^{i(h\omega - E + i\gamma(s))t} - \int_0^\infty ds e^{i(h\omega + E + i\gamma(s))t} \right].$$

(1)

where, the subscripts $c$ and $v$ indicate the conduction and valence bands, respectively, $E = E_{cv}(k)$ is the energy difference between a pair of bands in $k$ space, $J_{cv}(E)$ is the joint density of states between the pair of bands, and $P_{cv}(E)$ is the weighted-average matrix element of the momentum operator. If we expand the $\gamma(s)$ in a power series in $s = i\hbar/t$, where $t$ is time, and retain only the first two terms of the expansion we obtain the following approximation:

$$\gamma(s) = \Gamma + \sigma^2 s.$$

(2)

If $\gamma(s)$ is replaced by $\Gamma$ in Eq. (1), then the broadening function $\Phi$ takes the form

$$\Phi_L(h\omega \pm E) = -i \int_0^\infty ds e^{i(h\omega \pm E + i\Gamma)t}.$$

(3)

This function after integration leads to the approximation which is usually referred to as Lorentzian broadening function,

$$\Phi_L(h\omega \pm E) = \frac{1}{h\omega \pm E + i\Gamma}.$$

(4)

It has been shown, however, that in the case of line broadening caused by electron-phonon and electron-impurities scattering a much better approximation for $\gamma(s)$ is a linear function of time $\gamma(s) = \sigma^2 s$. This approximation is usually referred to as Gaussian broadening because of the Gaussian time decay in Eq. (1). This yields

$$\Phi_G(h\omega \pm E) = -i \int_0^\infty ds e^{i(h\omega \pm E + i\sigma^2 t)s},$$

(5)

which after integration gives

$$\Phi_G(h\omega \pm E) = -i \frac{\sqrt{\pi}}{2\sigma} e^{-[(h\omega \pm E)^2/4\sigma^2]} \left[ 1 + \text{erf}\left( \frac{h\omega \pm E}{2\sigma} \right) \right].$$

(6)

For the case of the Gaussian broadening, however, the integration of Eq. (1) in the energy domain cannot be done analytically in closed form.

Now, let us compare the imaginary parts of the broadening functions given by Eq. (4) and Eq. (6).

$$\text{Im}[\Phi_L(h\omega \pm E)] = \frac{\Gamma}{(h\omega \pm E)^2 + \Gamma^2},$$

(7)

$$\text{Im}[\Phi_G(h\omega \pm E)] = \frac{\sqrt{\pi}}{2\sigma} \exp\left( -\frac{(h\omega \pm E)^2}{4\sigma^2} \right).$$

(8)

Equations (7) and (8) are plotted in Fig. 1, where the same strength and full width at half maximum have been assumed for both broadening functions. Figure 1 shows that the Lorentzian broadening function has higher and extended wings compared to the Gaussian one. It is therefore clear that an optical dielectric function calculated using the approximation (4) will also have extended absorption tails $[\text{in } \varepsilon_{r2}(\omega)]$

![FIG. 1. Comparison of different broadening functions; Lorentzian broadening function (solid line); Lorentzian function with frequency-dependent damping constant (broken lines); Gaussian broadening function (open circles).](image)
in comparison with $\varepsilon_2(\omega)$ calculated using the approxima-
tion (6). This is always true regardless of the functional form of the
joint density of states function. Accordingly, all the models based on the Lorentzian broadening function exhibit exces-
sive absorption near the fundamental band gap. For ex-
ample, the $\varepsilon_2(\omega)$ values calculated using the model of Adac-
chi exceed the experimental data up to two orders in mag-
nitude in the region of critical point energy $E_0$. In their model
incorporating Lorentzian broadening Kim et al.31 replaced the
damping constant $\Gamma$ with the frequency dependent damp-
ing constant $\Gamma'$ given by
$$\Gamma' = \Gamma \exp\left[-\frac{1}{\Gamma} \frac{(\hbar \omega - E_0)^2}{\alpha}\right].$$

Thus, they obtained the analytic function which closely re-
sembles the numerical result for the Gaussian broadening
case, if suitable values for $\alpha$ are assumed. This, however,
introduces an additional parameter per each transition be-
sides the strength, energy, and linewidth. This additional pa-
rameter $\alpha$, allows for a continuous change of the lineshapes
ranging from a purely Lorentzian (for $\alpha=0$) to nearly
Gaussian (for $\alpha=0.30$), as shown in Fig. 1. Therefore a
range of broadening function approximations with similar
kernels and different wings can be obtained using Eq. (9).
This applies equally well, not only to Kim’s model, but to all
models with Lorentzian damping, such as the model of Ada-
chi.

We used this fact to change the shape of the absorption
lines of all the seven transitions in our model by replacing
the damping constants in Eqs. (10) to (18) by the frequency
dependent broadening parameter $\Gamma'$. This, in turn, has en-
abled us to eliminate the spurious absorption in the $E_0$ CP
region.

### III. MODEL FOR THE DIELECTRIC FUNCTION

We start with the outline of Adachi’s composite model.29
We then replace the damping constant $\Gamma$ in Eqs. (10)–(18)
by the frequency-dependent damping constant $\Gamma'$ given by
Eq. (9). The optical dielectric constant is then represented by
the sum of several terms describing transitions at CPs in the
joint density of states labelled $E_0$, $E_0 + \Delta_0$, $E_1$, $E_1 + \Delta_1$,
$E_1'$, $E_2(X)$, and $E_2(\Sigma)$.

#### A. $E_0$ and $E_0 + \Delta_0$ transitions

The $E_0$ and $E_0 + \Delta_0$ transitions occur in the center of the
Brillouin zone (BZ). Assuming the parabolic bands, Adachi
obtains29 contribution of these gaps to $\varepsilon_1(\omega)$
$$\varepsilon_1(\omega) = A E_0^{3/2} \left\{ f(\chi_0) + \frac{1}{2} \left( \frac{E_0}{E_0 + \Delta_0} \right)^{3/2} f(\chi_{s.o.}) \right\},$$
where
$$f(y) = y^{-2} [2 - (1 + y)^{1/2} - (1 - y)^{1/2}],$$
$$\chi_0 = \frac{\hbar \omega + i \Gamma_0}{E_0},$$
$$\chi_{s.o.} = \frac{\hbar \omega + i \Gamma_0}{E_0 + \Delta_0},$$
$$\hbar \omega + i \Gamma_0,$$
where $A$ and $\Gamma_0$ are the strength and damping constant of the
$E_0$ and $E_0 + \Delta_0$ transitions, respectively.

#### B. $E_1$ and $E_1 + \Delta_1$ transitions

The $E_1$ critical point in the joint density of states corre-
sponds to the transition at the L point in the Brillouin zone.
Taking the matrix element to be constant with respect to
energy Adachi obtained the following
$$\varepsilon_1^1(\omega) = -B_1 \chi_1^{-2} \ln(1 - \chi_1^{-2}) - B_1 \chi_1^{-2} \ln(1 - \chi_1^{-2}),$$
with
$$\chi_1 = \frac{\hbar \omega + i \Gamma_1}{E_1},$$
$$\chi_1 = \frac{\hbar \omega + i \Gamma_1}{E_1 + \Delta_1},$$
where the $B_1$ ($B_2 \chi$) and $\Gamma_1$ are, respectively, the strength
and damping constant of the $E_1$ ($E_1 + \Delta_1$) transitions.

The discrete series of excitons at the $E_1$ and
$E_1 + \Delta_1$ CPs can be written, assuming the Lorentzian line
shape in the form27,29
$$\varepsilon_1^I(\omega) = \sum_{n=1}^{\infty} \frac{1}{(2n-1)^2} \left( \frac{B_1}{E_1 - \left( G_1/(2n-1)^2 \right)} - \hbar \omega - i \Gamma_1 \right) \chi$$
$$+ \frac{B_2 \chi}{E_1 + \Delta_1 - \left( G_1/(2n-1)^2 \right)} - \hbar \omega - i \Gamma_1,$$
where $B_1$ ($B_2 \chi$) is the strength and $G_1$ ($G_2 \chi$) is the Rydberg
energy of the $E_1$ ($E_1 + \Delta_1$) exciton. Here we assumed that
$G_1 = G_2 \chi = 0$.

#### C. $E_1'$, $E_2(X)$, and $E_2(\Sigma)$ transitions

The origin of the transitions $E_1'$, $E_2(X)$, and $E_2(\Sigma)$ is
still an open question. These features in the spectrum are
adequately modeled using three damped harmonic oscillators
$(j = 1,2,3)$ with energy $E_j$, strength $f_{E_j} = C_{E_j} E_j^{2}$ and
damping constant $\Gamma_{E_j}$
$$\varepsilon_1^V(\omega) = \varepsilon_s + \sum_{j=1}^{3} \frac{C_{E_j} E_j^{2}}{E_j^2 - (\hbar \omega)^2 - i \hbar \omega \Gamma_{E_j}},$$
where $\varepsilon_s$ is the high-frequency dielectric constant containing
the contribution of higher-lying transitions.

#### D. Complete model for the dielectric function

Summing over all of the contributions to $\varepsilon_1(\omega)$ given by
Eqs. (10), (14), (17), and (18) yields the complete model for
the dielectric function
$$\varepsilon_1(\omega) = \varepsilon_1^l(\omega) + \varepsilon_1^m(\omega) + \varepsilon_1^m(\omega) + \varepsilon_1^V(\omega).$$

Now we substitute the $\Gamma'(\omega)$ for $\Gamma$ in Eq. (19).
TABLE I. Values of the critical-point energies $E_i$ for GaAs and AlAs from Ref. 32.

<table>
<thead>
<tr>
<th>$E_i$ (eV)</th>
<th>GaAs</th>
<th>AlAs</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_0$</td>
<td>1.410</td>
<td>2.993</td>
</tr>
<tr>
<td>$E_0 + \Delta_0$</td>
<td>1.746</td>
<td>3.201</td>
</tr>
<tr>
<td>$E_1$</td>
<td>2.926</td>
<td>3.888</td>
</tr>
<tr>
<td>$E_1 + \Delta_1$</td>
<td>3.170</td>
<td>4.087</td>
</tr>
</tbody>
</table>

IV. RESULTS AND DISCUSSION

A. Fitting procedure

The position of the four lowest-lying-transitions ($E_0$, $E_0 + \Delta_0$, $E_1$, and $E_1 + \Delta_1$) is known with accuracy from the excellent studies of Lautenschlager et al.,35 Garriga et al.,36,37 and Kim et al.38,31,32 The values of these CP energies are listed in Table I, following the Ref. 32, and they do not represent adjustable parameters of the fit.

Ozaki and Adachi29 used four oscillators in Eq. (18) to model transitions $E_0$, $E_2(X)$, and $E_2(\Sigma)$. We have found, however, that these features in the spectrum can be modelled with sufficient accuracy by only three oscillators. Therefore, we use five different values for damping constant in our model; $\Gamma_0$ and $\Gamma_1$, for the four lowest-lying transitions ($E_0$, $E_0 + \Delta_0$, $E_1$, and $E_1 + \Delta_1$) and $\Gamma_{E_1}$, $\Gamma_{E_2(X)}$, and $\Gamma_{E_2(\Sigma)}$ for transitions described by Eq. (18). By introducing the lineshape parameter $\alpha$, the number of fitting parameters is increased by five. However, we found that $\alpha E_{0}^{-\alpha} \alpha E_{2(X)}^{-\alpha} \alpha E_{2(\Sigma)}^{-\alpha}$, and that one can use the same lineshape parameter for all transitions in Eq. (18). This leaves only 20 fitting parameters in our model, in comparison with 23 that are used in Ref. 29.

No attempt has been made here to constrain the values of the strengths and linewidths in the fitting procedure, even by an order of magnitude. The following merit function was used:

$$
\chi^2 = \sum_{i=1}^{N} \left[ \frac{\varepsilon_{i1}(\omega_i) - \varepsilon_{i1}^{\text{exp}}(\omega_i)}{\varepsilon_{i1}^{\text{exp}}(\omega_i)} + \frac{\varepsilon_{i2}(\omega_i) - \varepsilon_{i2}^{\text{exp}}(\omega_i)}{\varepsilon_{i2}^{\text{exp}}(\omega_i)} \right]^2 .
$$

To minimize the merit (or cost) function we use the acceptance-probability-controlled simulated annealing (APCSA) algorithm (described in detail in Ref. 34) which was specifically designed for solving parameter estimation problems. This algorithm has proved to be fully insensitive to initial parameters-values, extremely efficient in escaping local minima, and shows faster convergence compared to adaptive-step classical simulated annealing with exponential cooling schedule. Optimal values for the model parameters, obtained from this algorithm, are listed in Table II for both GaAs and AlAs.

B. GaAs

In applying the model described in Sec. III to GaAs, fit has been made to the data published in the Handbook of Optical Constants of Solids I.39 Figures 2 and 3 show the comparison between the dielectric function of GaAs calculated using our model (solid line), Adachi’s model29 with Lorentzian broadening (dashed line) and experiment. It can be seen that our model produces a better fit to experimental data, in particular in the $E_0$ critical point region and below. Poor fit of Adachi’s model to to $\varepsilon_{i2}^{\text{exp}}(\omega)$ around $E_0$ can be attributed to the wings of the absorption lines above the $E_1$ critical point.
C. AlAs

The experimental data for intrinsic AlAs at room temperature used in this article are shown in Fig. 4. These data were taken from Herzinger et al.\textsuperscript{14} for the region 0.50–3.00 eV, and from Garriga et al.\textsuperscript{37} for the region 3.00–5.60 eV. Selected experimental data points from other sources\textsuperscript{36,40–43} are shown for comparison.

Garriga et al.\textsuperscript{37} have measured the dielectric constant of AlAs using a heterostructure specifically designed to provide accurate results above the $E_0$, and in the $E_2$ critical point spectral region. Study of Herzinger et al.\textsuperscript{14} emphasizes on accurate values of dielectric function below the $E_0$ critical point, and is more tolerant in the UV region. Bulk AlAs prism measurements of Fern and Onton\textsuperscript{44} in the region 0.56–2.05 eV (see inset to Fig. 4) are in excellent agreement with the measurements of Herzinger et al.\textsuperscript{14}

In Figs. 5 and 6 the optical dielectric function of AlAs calculated using our model (solid line) is compared to experiment and to the Adachi’s model with Lorentzian broadening (dashed line). The inset to Fig. 6 shows region at about $E_0$, where the effect of the Gaussian-like broadening approximation on the shape of the $\varepsilon_2(\omega)$ is most pronounced.

V. CONCLUSION

This article has discussed the significance of using the proper broadening-function approximation in models for the optical dielectric function of GaAs and AlAs. It has been shown that major discrepancies between the modelled and experimental dielectric functions (in the region of the fundamental band gap) can be attributed to the broadening effect. This holds regardless of the functional form of the joint density of states function. The improvement in the recent model by Ozaki and Adachi\textsuperscript{29} has been achieved by incorporating Gaussian-like broadening approximation in place of the originally used Lorentzian broadening. In this way a consistent and comparatively simple analytic model has been ob-

FIG. 3. The imaginary part $\varepsilon_2$ of the optical dielectric function of GaAs. The solid line shows the values calculated using our model. Broken line corresponds to Adachi model using the Lorentzian broadening approximation, where open circles indicate experimental data. The inset shows the fit to $\varepsilon_2(\omega)$ around the CP energy $E_o$.

FIG. 4. Refractive index and the extinction coefficient for AlAs. The solid curve is from Herzinger et al. (see Ref. 14). The chain line is from Garriga et al. (see Ref. 37). Also shown are selected experimental data points from: Perkowitz et al. (see Ref. 41) ($\triangle$), Fern and Onton (see Ref. 44) ($\bullet$), Adachi (see Ref. 43) ($\circ$), Monemar (see Ref. 42) ($\nabla$), and Garriga et al. (see Ref. 36) ($\square$).

FIG. 5. The real part $\varepsilon_1$ of the optical dielectric function of AlAs. The solid line shows the values calculated using our model. Broken line corresponds to Adachi’s model using the Lorentzian broadening, where the open circles indicate experimental data.
tained, which accurately describes the dielectric function of GaAs and AlAs in a wide spectral range between 0.1 and 6 eV.

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