Analytical Model for Δn and α Effects in GaAs

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Introduction

Index perturbation (Δn) and light absorption (α) effects within a GaAs waveguide are modeled as functions of applied bias (V_{bias}), wavelength (λ or photon energy E_γ), and carrier concentrations (N and P).

To provide a full solution, these effects must be applied to a physically modeled system including the waveguide optical mode, DC electric field distribution, and carrier distribution:

$$\Delta n_{TE} = \frac{\int I(r)\ \left(\Delta n_{EO}(E_j(r)) + \Delta n_{FC}(N(r),P(r))\right)\ dr}{\int I(r)\ dr}$$

$$\alpha = \frac{\int I(r)\ \left(\alpha_{EA}(E_j(r)) + \alpha_{FC}(N(r),P(r))\right)\ dr}{\int I(r)\ dr}$$

$$\{r\} = \{x,y\} = \text{cross-section perpendicular to direction of optical propagation}$$
$$I(r) = \text{optical intensity}$$
$$\{N(r),P(r)\} = \text{carrier density}$$
$$E_j(r) = \hat{z}\ \text{component of DC electric field}$$

Potential tools to determine these distributions are Lumerical MODE (optical) and Lumerical CHARGE (electrical), or similar finite element physics simulation software such as COMSOL. Finding and applying these solutions are beyond the scope of this document.

Assumed System

Effects are modeled assuming a p-i-n GaAs epitaxy, with a DC electric field (amplitude E_j) created along the vertical (surface-normal) direction by applying a bias (V_{bias}) across the p-i-n junction, and with light propagating through a waveguide perpendicular to this field. Unless specified, the optical mode in the waveguide is assumed to be TE polarization ($\vec{E}_{opt}$ perpendicular to both the propagation direction and DC field).

Definitions

$$E_\gamma = h\nu = \hbar\omega = \text{photon energy}$$
$$E_g = \text{material bandgap; } 1.424\text{ eV for GaAs}$$
$$E_j = E_j^1 * (V_0 - V_{bias}) \approx E_j^0 - E_j^1 * V_{bias} = \text{DC electric field in vertical direction}$$
$$\alpha = \text{absorption per length, via } P(z) \propto \exp(-\alpha\ z)$$

Index Perturbation Effects

$$\Delta n = \text{change in refractive index}$$
$$\Delta\phi = 2\ \pi\ \Delta n\ L/\lambda$$

Linear Electro-Optic (LEO)

Same as the *Pockels effect*: an induced birefringence.

$$\Delta\left(\frac{1}{n^2}\right) = \pm r_{41}\ |E_j|$$

r_{41} is only nonzero for TE polarization, and the expression is positive for propagation along **`[1 1 0]`** and negative for propagation along **`[1 -1 0]`**. r_{41} scales as $A - B/n(\lambda)^2$ below the bandgap[1].

LEO Coefficient

From fits to literature values for GaAs, including data from Berseth [2] and Faist[3]:

$$r_{41} = (7.788 - 72.16/n^2) * 10^{-10}\ [\text{cm/V}]$$

Quadratic EO (QEO)

Also known as the *Franz-Keldysh* or *band bending* effect.

With an applied electric field, the band edges are tilted, thus increasing the overlap of the electron and hole wavefunctions in the conduction and valence bands - increasing the tunneling probability. This shifts the absorption edge to lower energies, or alternatively creates exponential tails in the absorption edge. Via the Kramers–Kronig (K-K) relations, this changes the refractive index below the absorption edge[4].

$$\Delta\left(\frac{1}{n^2}\right) = R(\lambda)\ |E_j|^2$$

There is a slight polarization dependence reported by some sources[3:1].

Note that the exact analytical solution (via K-K) is not quite $|E_j|^2$ [5].

QEO Coefficient

From Mendoza-Alvarez[4:1] for GaAs up to 1.55 μm,

$$R(\lambda) = 3.45 * 10^{-17}\ \exp(3\ (\mu\mathrm{m}^3)/\lambda^3)\ \mathrm{cm}^2\ \mathrm{V}^{-2}$$

From Faist[6],

$$R = \frac{A\ E_\gamma^2}{n^4\ (E_g^2 - E_\gamma^2)^2},\ A = 85 * 10^{-16}\ \mathrm{eV}^2\ \mathrm{cm}^2\ \mathrm{V}^{-2}$$

Note that these two dispersion relations do not have the same form! These two equations bracket reported values in literature, with fits of either form giving good agreement. As Faist's model only has a single parameter, that is adopted for simplicity, with coefficients:

$$A_{TE} = 167.7 * 10^{-16}\ \mathrm{cm}^2\ \mathrm{V}^{-2}$$
$$A_{TM} = 198.5 * 10^{-16}\ \mathrm{cm}^2\ \mathrm{V}^{-2}$$

Quantum-confined Stark Effect (QCSE)

For quantum well (QW) systems, this is a similar effect that is also quadratic in E_j. Essentially the same as the Franz-Keldysh effect, it is instead applied to the electron and hole wavefunctions confined in a quantum well. There is no general solution - it must be solved with $k \cdot p$ (or similar) models and the K-K relation[7]. The Lumerical MQW product can also solve this directly with **`mqwindex`**.

DC Kerr Effect

This effect is rarely addressed. While nonzero in GaAs, it is $< 1 * 10^{-7}$ the fraction of the other EO effects, so can safely be neglected.

$$\Delta n_{Kerr} = \frac{3\ \mathrm{X}^{(3)}\ E_j^2}{2\ n}$$

For GaAs, $\mathrm{X}^{(3)} \lesssim 3 \cdot 10^{-15}\ \mathrm{cm}^2/\mathrm{V}^2$ at 1030nm[8].

Free Carrier Plasma (FP or PL)

The change of free carrier absorption in the conduction or valence band alters the refractive index via K-K. Index increases when carriers decrease.

From Faist[6:1], intervalence band absorption:

$$\Delta n_{FP} = -2.9 * 10^{-22}\ \frac{P}{E_\gamma^2}$$

Plus scattering by free carriers:

$$\Delta n_{PL} = -\frac{n}{2}(\frac{\nu_p}{\nu_\gamma})^2,\ \nu_p^2 = \frac{q^2\ \{N, P\}}{\epsilon\ m_{n,p}^*}$$

Given effective masses from **`ioffe.ru`**:

$$m_c = 0.063\ m_0, m_{lh} = 0.082\ m_0, m_{hh} = 0.51\ m_0$$

This reduces to:

$$\Delta n_{PL} = -\frac{\{N, P\}}{n\ E_\gamma^2}\ \left(\frac{h^2\ q^2}{8\ \pi^2\ \epsilon_0\ m^*}\right)$$
$$\Delta n_{PL} = -\frac{1}{n\ E_\gamma^2}\ \left(N * 1.09 * 10^{-20}\ [\mathrm{cm}^3\ \mathrm{eV}^2] + P * 1.35 * 10^{-21}\ [\mathrm{cm}^3\ \mathrm{eV}^2]\right)$$

Comparing to Stern[9] (noted as approximate with up to 50% error by Mendoza-Alvarez[4:2]), this is similar for N, and also similar for P *if light holes are neglected*. Comparing to Faist's total carrier contribution formula (not printed), neglecting light holes seems to be the correct interpretation.

Band-gap Shift (BS)

A combination of Band-gap Shrinkage (BGS) and Band Filling (BF) shifting the fundamental absorption edge, thus altering the index via K-K.

From Faist[6:2] for GaAs at room temperature,

$$\Delta n_{BF} = -2.92 * 10^{-21}\ \frac{N + P}{E_g^2 - E_\gamma^2}$$
$$\Delta n_{BGS} = +\frac{(b_n\ N + b_p\ P)}{E_g^2 - E_\gamma^2}$$
$$b_n = 8.9 * 10^{-22}\ \mathrm{cm}^3\ \mathrm{eV}^2,\ b_p = 1.42 * 10^{-21}\ \mathrm{cm}^3\ \mathrm{eV}^2$$

Compared to Lee[10] near 1 μm, the n-type coefficients are similar, but p-type coefficients differ by 3x. This discrepency is noted by Lee *et al.*.

Total Index Perturbation

Electro-Optic Effects

Considering only the LEO and QEO effects,

$$\Delta\left(\frac{1}{n^2}\right) = \left(\frac{1}{n + \Delta n_{EO}}\right)^2 - \left(\frac{1}{n}\right)^2 = \pm r_{41}|E_j| + R\,|E_j|^2$$

$$\Delta n_{EO} = n\left(\frac{1}{\sqrt{1 + n^2\ (r_{41}|E_j| + R\,|E_j|^2)}} - 1\right)$$

Expanding quadratically in E_j and discarding higher order r_{41} and R terms,

$$\Delta n_{EO} \approx -\frac{n^3}{2}(\pm r_{41}\,|E_j| + R\,|E_j|^2)$$

However, the electric field is $E_j \approx E_j^0 - E_j^1 * V_{bias}$. Expanding to quadratic V_{bias} and discarding higher order r_{41} and R terms,

$$\Delta n_{EO} \approx -\frac{n^3}{2}\left((\pm r_{41}\,E_{j0} + R\,E_{j0}^2)\;+\;(\pm r_{41} + 2\,R\,E_j^0)\,(E_j^1\,V_{bias})\;+\;(R)\,(E_j^1\,V_{bias})^2\right)$$

$$r_{41} = (7.788 - 72.16/n^2) * 10^{-10}\ \mathrm{cm/V}$$

$$R = \frac{A\,E_\gamma^2}{n^4\,(E_g^2 - E_\gamma^2)^2},\ A_{TE} = 167.7 * 10^{-16}\ cm^2\ \mathrm{V}^{-2},\ A_{TM} = 198.5 * 10^{-16}\ cm^2\ \mathrm{V}^{-2}$$

Note that the linear-in-V_{bias} term now also depends on R - so the linear term will both be higher than naively expected, and will be nonzero for TM modes.

Free Carrier Effects

Simply summing the listed effects:

$$\Delta n_{FC} = D_n\,N + D_p\,P$$

$$D_n = -\left(\frac{1.09 * 10^{-20}}{n\,E_\gamma^2} + \frac{2.03 * 10^{-21}}{E_g^2 - E_\gamma^2}\right)\ \mathrm{eV}^2\ cm^3,$$

$$D_p = -\left(\frac{2.9 * 10^{-22}}{E_\gamma^2} + \frac{1.35 * 10^{-21}}{n\,E_\gamma^2} + \frac{1.50 * 10^{-21}}{E_g^2 - E_\gamma^2}\right)\ \mathrm{eV}^2\ cm^3$$

More detailed calculations are performed by Huang [11] [12], but with nontrivial formulas involving band-structure integrations.

Optical Absorption Effects

There are two major sources of absorption important for modeling: free carrier absorption, present where the optical field overlaps free carriers, and electroabsorption from the Franz-Keldysh effect, where the DC electric field across the p-i-n junction bends the bands and thus shifts the absorption edge closer to the operating wavelength.

Free Carrier Absorption

The simple Drude model for free carrier absorption is[13]:

$$\alpha_{FC} = \frac{q^3\,h^2\,N}{4\pi^2\,\mu\,(m^*)^2\,n\,\epsilon_0\,c\,E_\gamma^2}$$

Good empirical electron mobility fits are available from Sotoodeh[14] (values in Sotoodeh Table 1):

$$\mu(N,T) = \mu_{min} + \frac{\mu_{max}\,(300\mathrm{K}/T)^{\theta_1} - \mu_{min}}{1 + \left(\frac{N}{N_{ref}\,(T/300\mathrm{K})^{\theta_2}}\right)^{\lambda}}$$

For GaAs at 300K, neglecting heavy holes (~1/40th), this evaluates to:

$$\mu_N = 500 + \frac{8900}{\left(1 + \left(\frac{N}{6*10^{16}}\right)^{0.394}\right)}\ [\mathrm{cm}^2\,\mathrm{V}^{-1}\,\mathrm{s}^{-1}],\ \mu_P = 20 + \frac{471.5}{\left(1 + \left(\frac{N}{1.48*10^{17}}\right)^{0.38}\right)}\ [\mathrm{cm}^2\,\mathrm{V}^{-1}\,\mathrm{s}^{-1}]$$

$$\alpha_{FC} = \frac{8.1 * 10^{-17}}{E_\gamma^2}\ [\mathrm{eV}^2\,\mathrm{cm}^4\,\mathrm{V}^{-1}\,\mathrm{s}^{-1}]\left(\frac{N}{0.063^2 * \mu_N(N)} + \frac{P}{0.082^2 * \mu_P(P)}\right)$$

Doping loss data

Alternatively, it may be possible to use an empirical fit to doped-GaAs loss instead of the Drude model. It is unclear if the loss from the doping is directly connected to free carrier absorption - sources of the data disagree:

- Spitzer[15], Johnson[16], and Babic[17] indicate the measured loss from doped GaAs is due to free carrier absorption
- Turner[18] indicates most is **not** free carrier absorption, especially P-type

It seems reasonable that absorption effects due to carrier concentration can be taken from this data.

A good empirical fit is:

$$\alpha_{FC} = 4.2\,[\mathrm{cm}^{-1}] * \left(\frac{N}{10^{18}\ cm^{-3}}\right)^{0.8} * (\lambda/\mu\mathrm{m})^{0.4}\;+\;8\,[\mathrm{cm}^{-1}] * \left(\frac{P}{10^{18}\ cm^{-3}}\right) * (\lambda/\mu\mathrm{m})^3$$

Comparing to the Drude model, the doped absorption loss is generally significantly lower by a factor of 0.8 - 6 for n-type, and 2.5 - 10 for p-type. The p-type scaling is similar between both, while the Drude model's n-doped scaling is higher w.r.t N and λ.

Overall, test data is needed to determine which model is more appropriate.

Electroabsorption

This is the same Franz-Keldysh effect responsible for the QEO index perturbation. Due to band bending, the effective bandgap is shifted closer to the operating wavelength, resulting in increased optical absorption at higher bias.

A simple parabolic band apoproximation from Tharmalingam and Callaway via Mendoza-Alvarez[4:3] and Alping[5:1] is:

$$\alpha_{EA} = \sum_j A_j \, |E_j|^{1/3} \, \left(\, \mathrm{AiryAi}'(\beta_j)^2 - \beta_j \, \mathrm{AiryAi}(\beta_j)^2 \, \right)$$

$$\beta_j = B_j \, (E_g - E_\gamma) \, |E_j|^{-2/3}$$

$$A_j = \frac{7.65 * 10^5}{n \, E_\gamma} \, (2\mu_j / m_0)^{4/3}$$

$$B_j = 1.1 * 10^5 \, (2\mu_j / m_0)^{1/3}$$

$$j = lh, hh; \; \mu_{lh} = 0.0369 \, m_0, \; \mu_{hh} = 0.0583 \, m_0$$

$$\text{Units in eV and cm}$$

Alping[5:2] multiplied the result by 1.30 to obtain agreement with measurements. Bennett[19] has more complex calculations involving nonparabolic band structures.

Comparison to Data

Compared to measured $\alpha(V_{bias})$ data, this model describes high-bias absorption very well at <= 1030 nm, and decently well above that. However, scaling is a problem. At 1030 nm, a very good fit has a scaling factor of ~1.2e-4; compare this to Alping's scaling of 1.3, and the 1e-4 can possibly be accounted for by missed unit scaling. Unfortunately this still underpredicts 980 nm loss and severely underpredicts >1030 nm loss. It is likely that the longer wavelengths are not Franz-Keldysh electroabsorption, so the apparently incorrect scaling can be neglected. It is also likely that other absorption effects are stronger at 980 nm - and the measured shapes do bear that out. Additionally, since this is a complicated function, the scaling factor is potentially present in a different coefficient - this has not been investigated.

For now, the simple parabolic band approximation **with a 1.2e-4 scaling factor** appears to be the best predictor of near-1 µm electroabsorption loss.

MQW systems

For MQW systems, full $k \cdot p$ or similar models are needed[7:1]. Lumerical MQW can also solve this directly with **`mqwindex`**.

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