Carrier Induced Change of Absorption Coefficient and Refractive Index of InP, AlGaAS, and InGaAs

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August 27, 2015

Summary

Carrier induced change of refractive index Δn of InP, AlGaAs, and InGaAs has been estimated. Bandfilling (Burstein-Moss effect), band-gap shrinkage, and free-carrier absorption (plasma effect) were included. Carrier concentrations of $10^{16}/cm^{-3}$ to $10^{19}/cm^{-3}$ and photon energies of 0.8 eV to 2.0 eV were considered. The two models I developed here were taken from two major references where the authors claimed the validity of the models had been verified through experimental data in the literature. Refractive index changes as large as 10^{-2} have been predicted for carrier concentrations over $10^{18}/cm^{-3}$.

This report gives a guidance in determining whether the carrier induced change should be included in the optical simulation of the devices. The results from this report indicates that carrier induced change is vital in our simulation.

Introduction

Free carrier induce index-change effect is traditionally treated by the classical Drude theory [1] where plasma effect by using a simple harmonic oscillator model is considered. Drude theory ignores the effects from ionized impurities and other carrier-related effect around the bandgap. This theory is only valid in very low doping and low optical frequency region. The results are not applicable in integrated-optics frequency region.

The lack of experimental Δn data due to free carriers in the literature turned people to Kramers-Kronig theory. Absorption data due to free carriers are available in the literature and can be used to verify the models. Once the formulation of carrier-induce absorption spectrum change, one can use Kramers-Kronig theory to predict the change of refractive index.

Quite a few paper appeared in the literature around 1990s including Huang's [2] and Bennett's [3] papers. Huang's paper looked at carrier effects on the change of refractive index for n-type AlGaAs, which would be useful for us to estimate n-contact. Bennett's paper broadly looked at III-V semiconductors when there are current injection, n-type doping and p-type doping. Therefore, Bennett's paper would be useful for estimating the intrinsic region of the photodetector as well as n- and p- contacts. I will proceed with Bennett's paper first, a model is developed first to match the results given in the paper using InP material parameters. Then I will use the model to predict absorption spectrum and refractive index of AlGaAs and InGaAs for MQW p-i-n photodetectors. Huang's paper is used to develop a model to look at n-junction of the photodetectors. Some comparisons will be made between these two models.

Theory and Results

Bandfilling Effect

A decrease in absorption for photon energies slightly above the nominal bandgap was observed when they are doped. This effect is most pronounced in semiconductors with small effective masses and band gaps. The effect, known as Burstein-Moss effect, can be explained by bandfilling effect [4] [5]. In the case of n-type semiconductors, the density of state in the conduction band is sufficiently low and a small number of electrons can fill the band to an appreciable depth. With the lowest energy states filled in the conduction band, electron from the valence band requires greater energy than nominal bandgap to be optically excited to the conduction band. Due to larger effective masses, p-type semiconductors have higher density of states. This effect is smaller for a given carrier concentration. *Because bandfilling is a results of free carriers, injection should be equivalent to doping, except that injection will result in bandfilling effects from both electrons and holes.*

If parabolic bands are assumed, optical absorption near the band gap in a direct bandgap semiconductor is given by the law:

$$\alpha_0(E) = \frac{C}{E}\sqrt{E - E_g}\ (E > E_g)$$

$$\alpha_0(E) = 0\ (E > E_g)$$

Where E is photon energy, E_g and C are bandgap energy and a constant, respectively. They both depend on material. The above equation can be written to explicitly take care of heavy and light holes:

$$\alpha_0(E) = \frac{C_{hh}}{E}\sqrt{E - E_g} + \frac{C_{lh}}{E}\sqrt{E - E_g}\ (E > E_g)$$

$$\alpha_0(E) = 0\ (E > E_g)$$

C_{hh} and C_{lh} are obtained from the parameter C. The reduce effective masses of the electron-hole pairs are given

$$\mu_{ehh} = \left(\frac{1}{m_e} + \frac{1}{m_{hh}}\right)^{-1}$$

$$\mu_{elh} = \left(\frac{1}{m_e} + \frac{1}{m_{lh}}\right)^{-1}$$

$$C_{hh} = C\left(\frac{\mu_{ehh}^{3/2}}{\mu_{ehh}^{3/2} + \mu_{elh}^{3/2}}\right)$$

$$C_{lh} = C\left(\frac{\mu_{elh}^{3/2}}{\mu_{ehh}^{3/2} + \mu_{elh}^{3/2}}\right)$$

In the case of bandfilling, there is finite probability that a state in the conduction band will be occupied by an electron and/or a state in the valence band will be empty of electron. If we denote an energy in the valence band by E_a and an energy in the conduction band by E_b, then the absorption is

$$\alpha(N, P, E) = \alpha_0(E)[f_v(E_a) - f_c(E_b)]$$

Where f(x) is Fermi-Dirac function. The change in absorption coefficient is

$$\Delta\alpha(N, P, E) = \alpha(N, P, E) - \alpha_0(E)$$

The change of refractive index is calculated through the Kramers-Kronig relation:

$$\Delta n(N, P, E) = \frac{2c\bar{h}}{e^2}\int_0^{\infty} \frac{\Delta\alpha(N, P, E')}{E'^2 - E^2}\, dE'$$

Table 1 Values of semiconductor parameters (T=300K)

	InP	GaAs	$In_{0.2}Ga_{0.8}As$
E_g (eV)	1.3507	1.424	0.8137
C ($cm^{-1}s^{-1/2}$)	3.0464e+12	2.4580e+12	1.1350e+12
C_{hh}($cm^{-1}s^{-1/2}$)	1.9246e+12	1.6317e+12	7.5797e+11
C_{lh}($cm^{-1}s^{-1/2}$)	1.1218e+12	8.2637e+11	3.7705e+11
ϵ_s	12.4	12.9	13.23
n	3.52	3.6	3.63
m_e (m_0)	0.075	0.0630	0.0545
m_{hh} (m_0)	0.56	0.5100	0.4900
m_{lh} (m_0)	0.12	0.0820	0.0708
m_{dh} (m_0)	0.6	0.5317	0.5078
μ_{ehh} (m_0)	0.066	0.0561	0.0491

μ_{elh} (m_0)	0.046	0.0356	0.0308
N_C (cm^{-3})	5.1442e+17	3.9604e+17	3.1883e+17
N_V (cm^{-3})	1.1537e+19	9.7100e+18	9.0624e+18
χ_{cr} (cm^{-3})	1.2902e+17	6.7919e+16	4.0780e+16

Note: in the above table, there is some discrepancy compared to the data provided in Bennett's paper [3]. In [3], only numbers are provided. In order to interpolate aluminum/indium concentration in AlGaAs/InGaAs, analytical expressions are used to estimate all the above parameters. For parameter C, there is the biggest discrepancy for InP's C parameter (25% smaller compared to [3]). All the other parameters are in good agreement with [3]. Comparison of InP calculation.

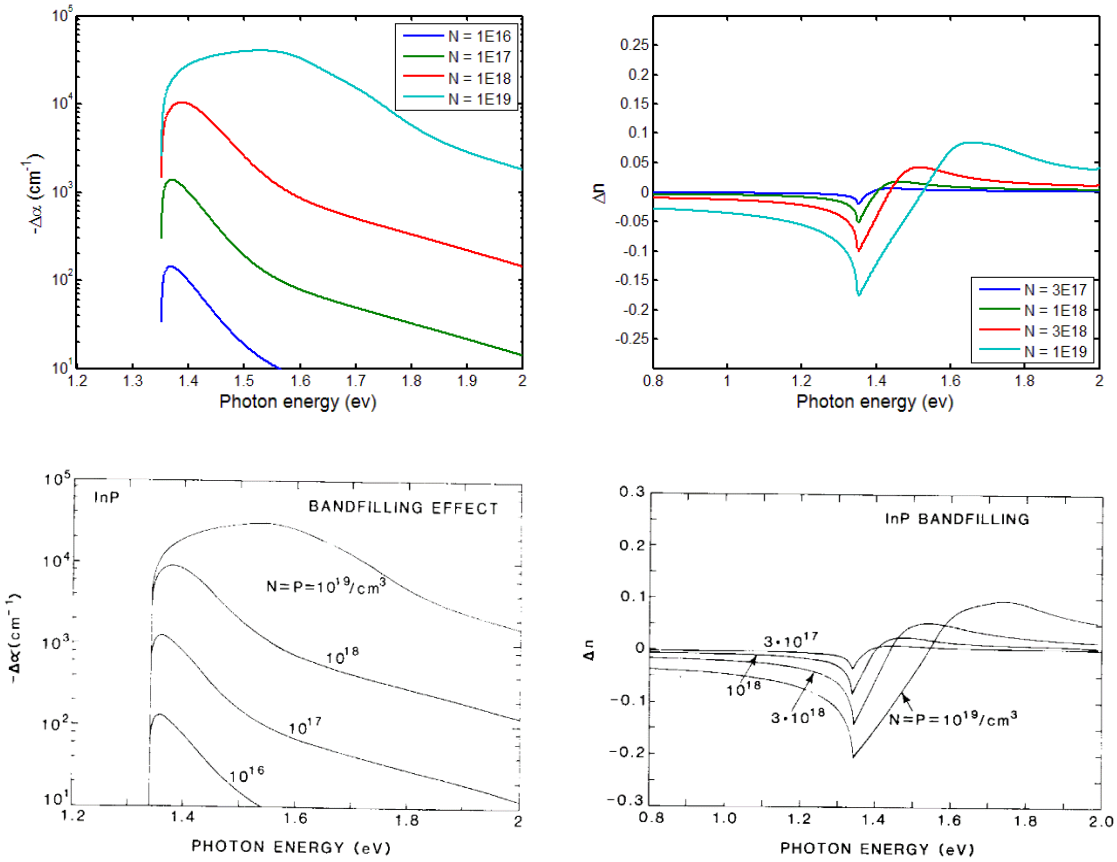


Figure 1 Comparison: (left) change in absorption due to electron-hole injection and the resulting bandfilling in InP; (right) change in refractive index due to bandfilling in InP.

The model is thus verified, and will be later applied to AlGaAs and InGaAs.

Bandgap Shrinkage

The basic mechanism is that injected electrons will occupy states at the bottom of the conduction band. If the concentration is large enough, the electron wavefunctions will overlap, forming a gas of interacting

particles. The electrons will repel one another by Coulomb forces. In addition, electrons with the same spin will avoid one another for statistical reasons. The net result is a screening of electrons and a decrease in their energies, lowering the energy of the conduction bandedge. A similar effect of holes increases the energy of valence bandedge.

Shrinkage effects are determined by free carrier density, and are independent of impurity concentration.

$$\Delta E_g(\chi) = \frac{\kappa}{\epsilon_s}(1 - \frac{\chi}{\chi_{cr}})^{1/3}, \chi > \chi_{cr}$$

$$\Delta E_g(\chi) = 0, \chi < \chi_{cr}$$

Where κ is a fitting parameter and χ_{cr} is critical concentration of free carriers. χ_{cr} is adopted to be 1.4 times the Mott critical density [6]

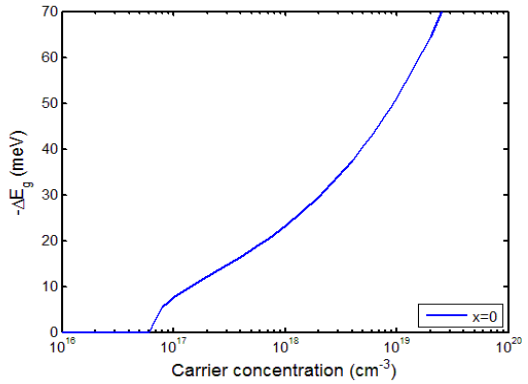
$$\chi_{cr} = 1.6 \times 10^{24}(\frac{m_e}{1.4\epsilon_s})^3$$

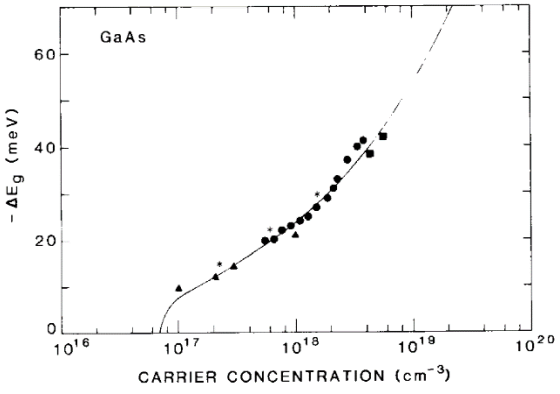
In the last equation, we used m_e instead of m_{hh} or m_{lh} because bandgap shrinkage effects start at a much lower concentration for electrons than holes. The above equation predicts $\chi_{cr} = 7 \times 10^{16}$cm^{-3} for n-type GaAs which is in good agreement with 5×10^{16} cm^{-3} [7]. Therefore, this formula is applied to InP and $In_{0.2}Ga_{0.8}As$ without further verification. The fitting parameter κ are 0.11, 0.125, and 0.14 for p-GaAs, n-GaAs and carrier injected electron-hole plasmas in GaAs.

Finally the bang gap shrinkage induce absorption change is

$$\Delta\alpha(\chi, E) = \frac{C}{E}\sqrt{E - E_g - \Delta E_g(\chi)} - \frac{C}{E}\sqrt{E - E_g}$$

The above equation predicts $\Delta\alpha$ will always be positive, largest near the bandgap and rapidly decrease for higher energy. With $\Delta\alpha$, Δn is calculated through Kramers-Kronig theory.





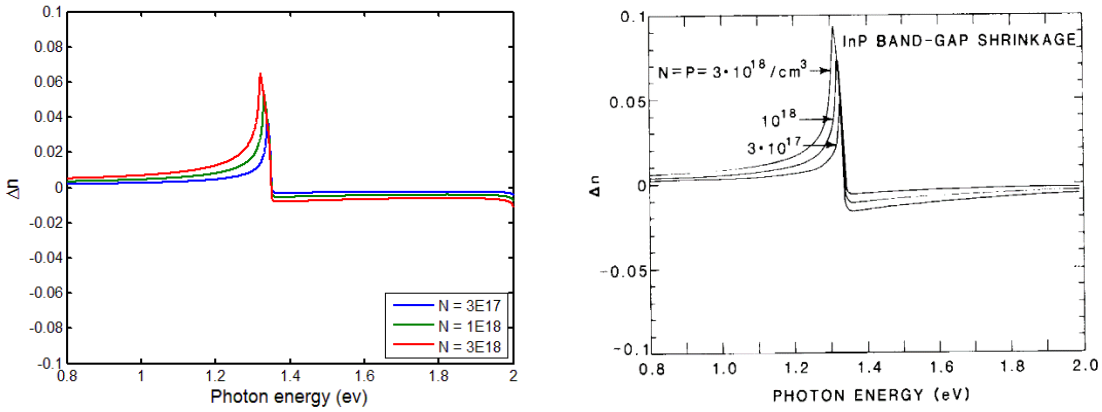


Figure 2 Comparison: (top) bandgap shrinkage in GaAs with κ =0.13 and $\chi_{cr} = 7 \times 10^{16}$; (bottom) change in refractive index of InP due to electron-hole injection and the resulting bandgap shrinkage.

Note, the simulated Δn is smaller than that from [3]. This is due to that C = 3.0464e+12 instead of 4.4e+12 in the paper. However, it was found that the expression used to calculate C gave more precise estimate for AlGaAs, this value is going to be used throughout the report.

The model is thus verified, and will be later applied to AlGaAs and InGaAs.

Free-Carrier Absorption

Thus far we have considered changes due to the interband absorption due to bandfilling and bandgap shrinkage. In addition, a free carrier can absorb a photon and move to a higher energy state within a band. In the Drude model, this is intraband free carrier absorption, also known as plasma effect. The corresponding change is [8]

$$\Delta n = \frac{-6.9 \times 10^{-22}}{nE^2}\left\{\frac{N}{m_e} + P\left(\frac{m_{hh}^{1/2} + m_{lh}^{1/2}}{m_{hh}^{3/2} + m_{lh}^{3/2}}\right)\right\}$$

The sign of Δn is always negative, hence it will add to bandfilling for energies below the bandgap. Because the E^2 dependence, the plasma effect increases as the photon energy decreases. On the other hand, both the bandfilling and bandgap shrinkage are the largest around the bandgap.

Combination of Effects

So far, the three effects, bandfilling, bandgap shrinkage, and free-carrier absorption, were assumed to be independent. However, the first two effects actually interplay a lot. Therefore, in calculating the combination of effects, bandfilling was based on the band gaps that had been obtained by considering bandgap shrinkage. The results agrees well with reference [3].

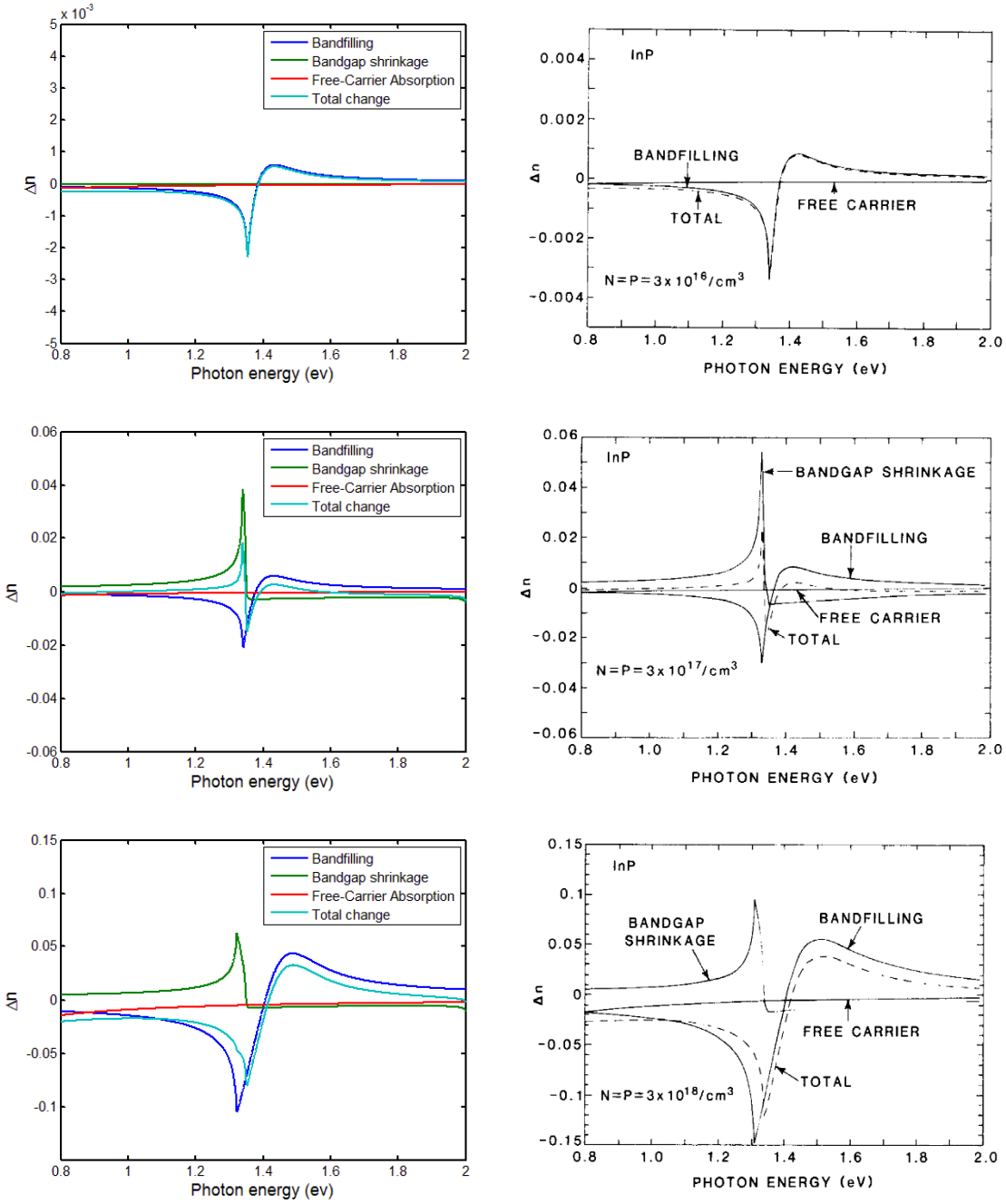


Figure 3 Predicted changes of refractive index from bandfilling, bandgap shrinkage, and free-carrier absorption. (top) N=P=3E16; (middle) N=P=3E17; (bottom) N=P=3E18.

In Figure 3 (top), the concentration is lower than the critical carrier density. Therefore, the bandgap shrinkage effect is zero throughout the photon energy range. The dominant effect is bandfilling effect. In Figure 3 (middle) where the carrier density is larger than χ_{cr}, the bandgap shrinkage effect comes into play and dominates over the other two effects. Near the bandgap, the total index change can be as high

as 0.02. In Figure 3 (bottom), as the carrier concentration increase to 3E18 cm^{-3}, the total index change can be as high as 0.1.

Doping Induced Effects

In the last section, we focus on carrier inject effects and charge neutrality is assumed, indicating N=P. If we are going to look at doping induced effects, we are going to use N only, i.e. N=3e18 cm^{-3}, and leave P at unintentional doping level, which is usually at 1e15 cm^{-3}. The opposite holds for p-type semiconductors, i.e. P=3e18 cm^{-3} and N=1e15 cm^{-3}.

Doping/Injection Induced Effects in AlGaAs and InGaAs

As we use $Al_{0.2}Ga_{0.8}As$ for n-contact layer and GaAs and $In_{0.2}Ga_{0.8}As$ for MQW layers, we need to know the carrier induced effects in order to calculate the absorption coefficient change (imaginary) and (real) refractive index change.

Table 2 Values of semiconductor parameters (T=300K)

	$Al_{0.2}Ga_{0.8}As$	GaAs	$In_{0.2}Ga_{0.8}As$
E_g (eV)	1.6734	1.424	0.8137
C ($cm^{-1}s^{-1/2}$)	4.0936e+12	2.4580e+12	1.1350e+12
C_{hh}($cm^{-1}s^{-1/2}$)	2.7437e+12	1.6317e+12	7.5797e+11
C_{lh}($cm^{-1}s^{-1/2}$)	1.3499e+12	8.2637e+11	3.7705e+11
ϵ_s	12.332	12.9	13.23
n	3.5117	3.6	3.63
m_e (m_0)	0.0796	0.0630	0.0545
m_{hh} (m_0)	0.5600	0.5100	0.4900
m_{lh} (m_0)	0.0956	0.0820	0.0708
m_{dh} (m_0)	0.5860	0.5317	0.5078
μ_{ehh} (m_0)	0.0697	0.0561	0.0491
μ_{elh} (m_0)	0.0434	0.0356	0.0308
N_C (cm^{-3})	5.6247e+17	3.9604e+17	3.1883e+17
N_V (cm^{-3})	1.1236e+19	9.7100e+18	9.0624e+18
χ_{cr} (cm^{-3})	1.5681e+17	6.7919e+16	4.0780e+16

n-doping $Al_{0.2}Ga_{0.8}As$

We inspect various doping levels for the martial $Al_{0.2}Ga_{0.8}As$. N will be varied and P is kept at unintentional doping level, which is usually at 5e15 cm^{-3}. We choose to see the N = 1e17, 5e17, 1e18, and 5e18 cm^{-3}.

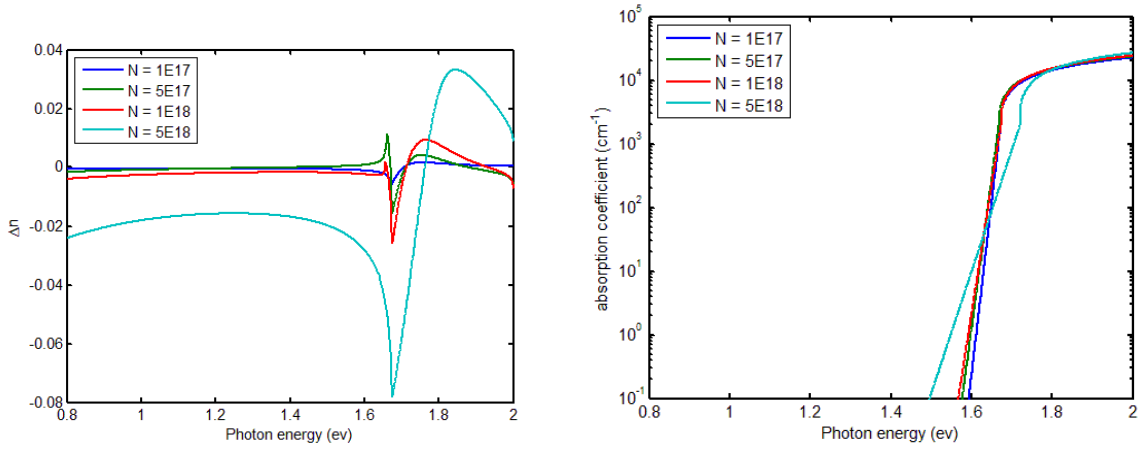


Figure 4 Change of refractive index and absorption coefficient of n-doped $Al_{0.2}Ga_{0.8}As$ for N = 1e17, 5e17, 1e18, and 5e18.

As can be seen from Figure 4, at doping concentration below N = 5e17, the doping induced refractive index change for photon energies 1.2eV to 1.5eV is negligible, so is absorption coefficient change. When voltages are applied to the contact, electrons are depleted, therefore change will be the opposite of what is shown in Figure 4. Overall, doping/inject induced RI change will be no more than 0.001, which can be seen from Figure 5.

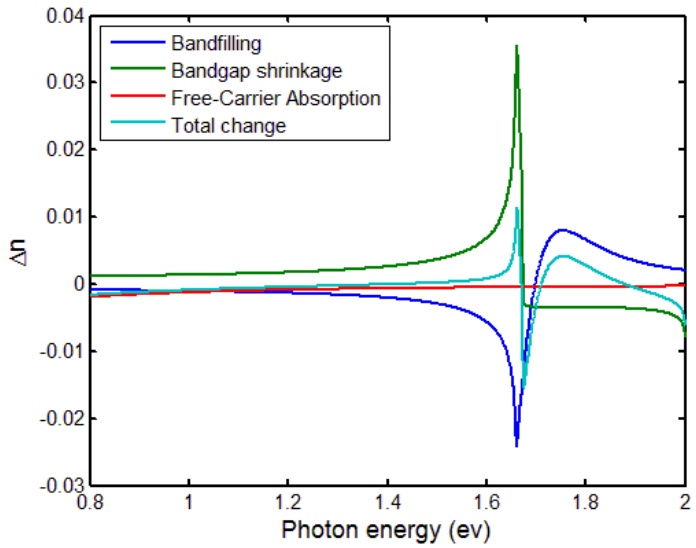


Figure 5 Predicted change of RI due to band filling, bandgap shrinkage, free carrier absorption, and total change of n-doped $Al_{0.2}Ga_{0.8}As$ for N= 5e17.

Carrier injection of GaAs and $In_{0.2}Ga_{0.8}As$ in the active region

Assuming charge neutrality in the active region, we have N = P, which has been used for developing model using InP. Again, we choose to see the N = P = 1e17, 5e17, 1e18, and 5e18 cm^{-3}.

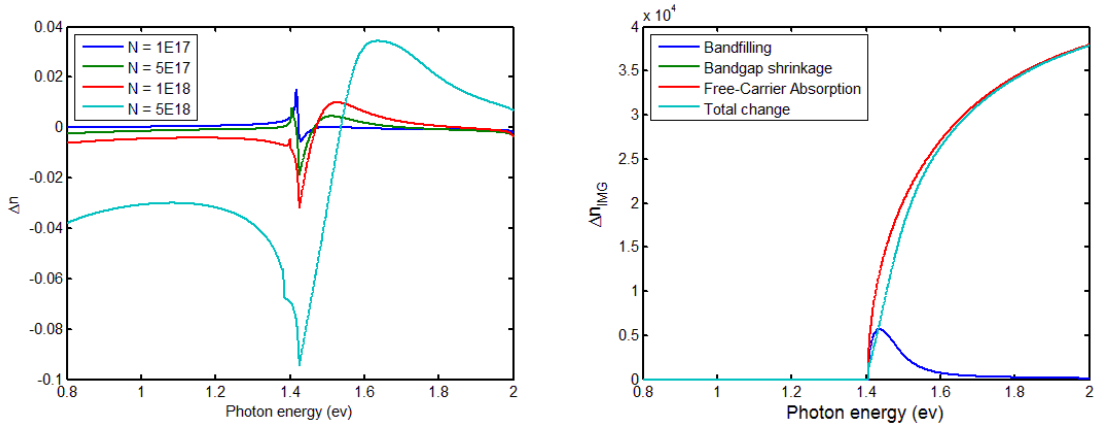


Figure 6 Change of refractive index and absorption coefficient of GaAs for N = P = 1e17, 5e17, 1e18, and 5e18.

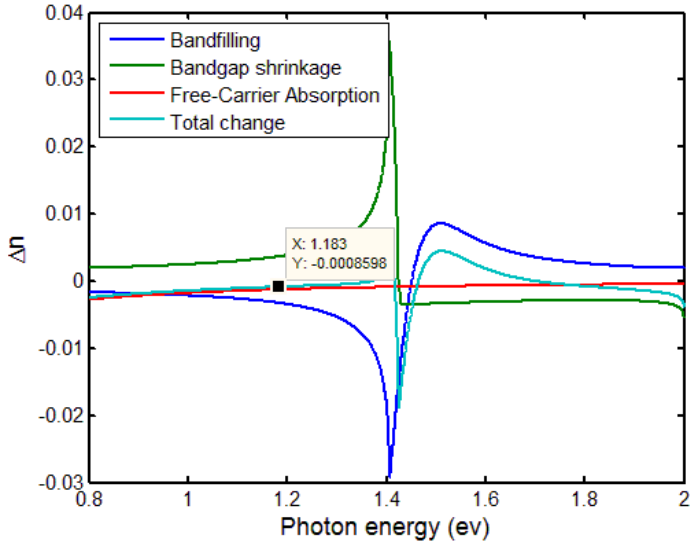


Figure 7 Predicted change of RI due to band filling, bandgap shrinkage, free carrier absorption, and total change of GaAs in the active region for N= 5e17.

Because InGaAs has narrow bandgap, we need to capture the change of RI around the bandgap. Therefore, the photon energy range has been changed.

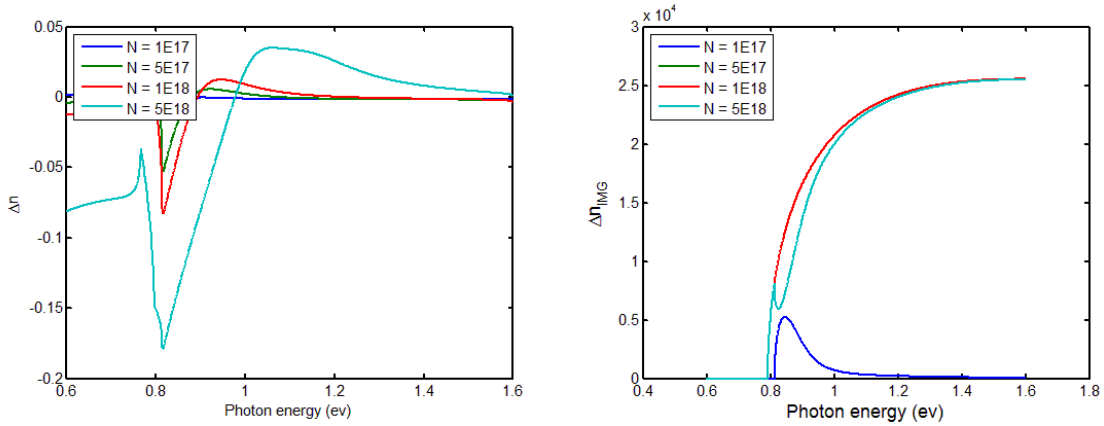


Figure 8 Change of refractive index and absorption coefficient of InGaAs for N = P = 1e17, 5e17, 1e18, and 5e18.

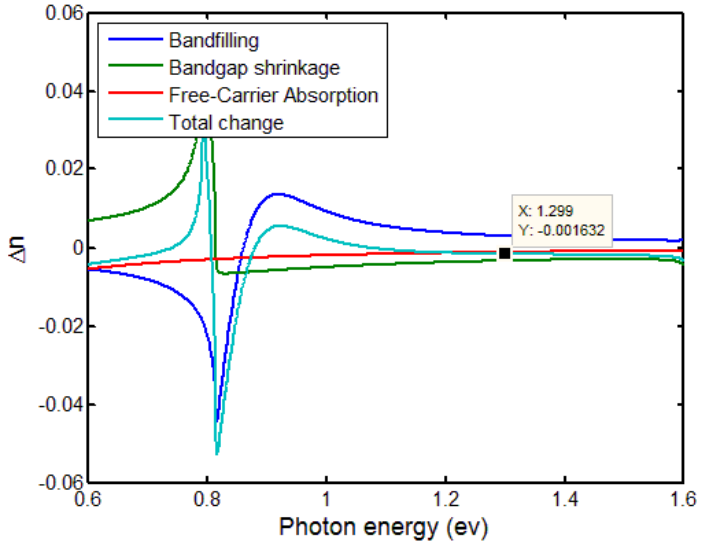


Figure 9 Predicted change of RI due to band filling, bandgap shrinkage, free carrier absorption, and total change of InGaAs in the active region for N= 5e17.

p-doping $Al_{0.3}Ga_{0.7}As$

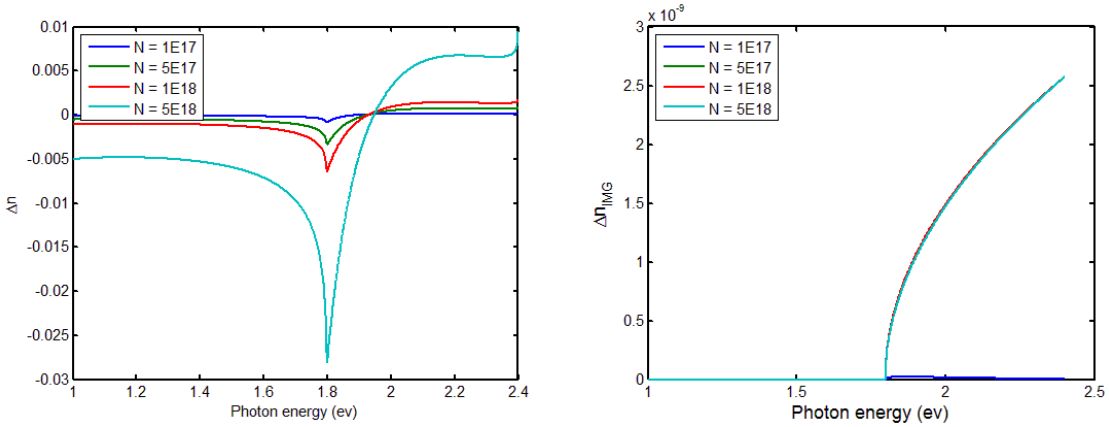


Figure 10 Change of refractive index and absorption coefficient of p-type AlGaAs for N = P = 1e17, 5e17, 1e18, and 5e18.

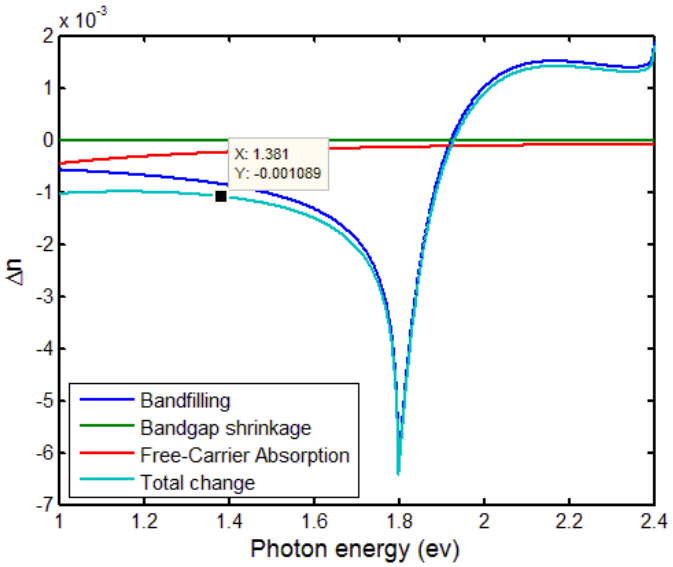


Figure 11 Predicted change of RI due to band filling, bandgap shrinkage, free carrier absorption, and total change of n-doped Al0.3Ga0.7As for N= 1e18.

Summary

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