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Many Body Theory of the Coupling of THz Radiation with Intersubband Excitations in GaAs/AlGaAs Quantum Well

*Aliyu, I. A., Turado, S., Bichi, T. S. and Ibrahim, U. B.

Kano University of Science and Technology, Wudil, Kano, Nigeria.

*Corresponding author's email: <u>ialiyufaragai@yahoo.co.uk</u>

ABSTRACT

The coupling of THz and Mid Infrared Radiation (TERA-MIR) with an optical excitation in semiconductor microcavities is the subject of increasing research interest. This can be attributed to their important in device's implementations and applications such as THz imaging, spectroscopy and detection of biological, explosive and hazardous materials. In this paper, we investigated the coupling of TE-THz mode with an intervalence band transition in GaAs/Al_{0.3}Ga_{0.7}As multiple quantum wells embedded in microcavities. Using mathematical modeling and numerical approach, applied to the valence subbands, the optical absorption of the model multiple quantum wells embedded in a microcavity resonator was determined. Simulation results for different carrier densities and dephasing are computed. The result shows clearly the influences dephasing and scattering mechanism as well as Coulomb's interactions on the energy dispersion of the terahertz Polari tonics.

Keywords:

Intersubbands transition, Interband transition, Optical absorption, THz polaritons.

INTRODUCTION

A semiconductor is a material characterize with valence and conduction bands, separated by an Energy gap (Eg). At absolute temperature the valence band is completely filled with electrons while the conduction band is empty. However as the temperature of the semiconductor increases, some of the ground state electrons gain more energy and move to the conduction band leaving behind a hole in the valence band. At thermal equilibrium the ratio of the total number of electrons in the conduction band to the total number of holes in the valence band is determine by (Wikipedia, 2012)

$$\frac{N_2}{N_1} = \frac{E_2 - E_1}{k_P T}$$
 (1)

where, N_2 , N_1 are the population (carrier) density of the conduction and valence bands respectively. k_B is the Boltzmann's constant, T is the thermodynamics temperature while $E_2 - E_1$ is the energy difference

between the conduction and valence bands. With recent development of quantum confined structures, electronics transition is also possible and controlled within the subbands of either conduction band or valence band, known as intersubband transition. This is achieved through quantum confinement.

Interband transitions

As stated, earlier electrons transition occurs between the valence band which is heavily populated and conduction band which is less populated, in a semiconductor material. This type of transition is called interband transition and it involves emission or absorption of photon in the process (Wikipedia, 2012, Dresselhaus, 2022). However, interband transition can be direct or indirect¹⁰. Depicted in Fig. 1 is a schematic diagram to indicate direct interband transition.



Figure 1: Schematic diagram showing direct interband transition

Intersubband transition

This occurs between subbands of a conduction band or valence band. Intersubband transition normally occurs in the far and mid infrared region, in confined structures, such as quantum wells. In Fig. 2, electrons transition between two subbands labeled n = 1 and n = 2 in an N-doped Quantum wells as depicted. In (a), it shows

photons absorption resulting in electrons transition from the lower subband, which is densely populated, to the upper subband (higher in energy). Emission of photon is achieved in (b) through transition from the excited subband to the lower subband.



Figure 2: Intersubband transition quantum well. (a) Absorption (b) emission process

The Absorption coefficient

The complex refractive index n and the dielectric of a medium are related by the equation

$$n(\omega) = \sqrt{\epsilon(\omega)} = \eta(\omega) + i\kappa(\omega) \tag{2}$$

Here η represent the real part of the refractive index and the term representing the imaginary part, κ is called the extinction coefficient (Pereira and Faragai, 2014) which measures the absorption of optical energy by the interacting medium.

Alternatively, one can write the following pair of equations

$$\eta^{2}(\omega) - \kappa^{2}(\omega) = \chi'(\omega) + 1$$
(3)
$$2\eta(\omega)\kappa(\omega) = \chi''(\omega)$$
(4)

The above pair of equations can be obtained from the Maxwell's equations for travelling electromagnetic wave in a dielectric medium. If we assumed a solution of the form;

$$E(r,t) = E_o e^{i(kz - \omega t)}$$
⁽⁵⁾

Where k is define the propagating wave number in the medium. Note that, a Fourier transform with respect to

time of the resulting Maxwell's equation was used in this case.

Now, the absorption coefficient, according to (Haug and Koch, 1994) is related to the extinction coefficient by $\alpha(\omega) = 2\kappa(\omega)$ (6)

By using Equations (2) - (4), and Eq. (6) the absorption coefficient can be represented as

$$\alpha(\omega) = \frac{\omega \chi''(\omega)}{c \eta(\omega)} \tag{7}$$

$$\eta(\omega) = \sqrt{\frac{1}{2} \left[(\chi'(\omega) + 1) \pm \sqrt{(\chi'(\omega) + 1)^2 + {\chi''}^2(\omega)} \right]}$$
(8)

Here, $\chi'(\omega)$ and χ'' represents respectively the real and imaginary part of the optical susceptibility.

MATERIALS AND METHODS Main Equations and Mathematical Models

The main equation describing both the polaritons and antipolaritons due to optical absorption and gain in the media is derived based on complex dielectric formalism. The first step involved self-evaluations of the complex optical susceptibility described by Equation (8) above. Based on many body non-equilibrium green function approaches, its summarized as in (Schmielau and Pereira Jr., 2009). Here only the resultant susceptibility is given;

$$\chi_{\delta\delta'}(\omega) = -\frac{\Lambda}{4\pi} \sum_{N} \left\{ \frac{1}{\omega - \omega_{\delta\delta'} + i\gamma_{\delta\delta'}} - \frac{1}{\omega + \omega_{\delta\delta'} + i\gamma_{\delta\delta'}} \right\} (9)$$

where N = 1,2,3,..., is the number of transition, ω and $\omega_{\delta\delta'}$ are the photon and transition frequency between subbands δ, δ' respectively, with $\delta \neq \delta' = 1,2,3,4$. A is the perturbed frequency, arisen from dipole coupling of the cavity modes and the intersubband transition, while $\gamma_{\delta\delta'}$ is the Lorentzian broadening term.

Next the susceptibility is adjusted using a fit parameters to the exact numerical solution for the GaAs/AlGaAs Qws with same population's differences between subbands for each transition. The dielectric function then is computed through the equation that relates it with the optical susceptibility.

$$\varepsilon(\omega) = \varepsilon_b + 4\pi\chi(\omega) \tag{10}$$

 ε_b , λ are respectively the background dielectric function and effective medium factor of the medium and details approach can be found in (Schmielau and Pereira Jr., 2009).

To described the propagation of an electric field in a dielectric medium, then one need a solution of wave

equation which can be derived from Maxwell equations and for a homogeneous medium is

$$\Delta E(\omega) + \frac{\omega^2}{c^2} \varepsilon(\omega) E(\omega) = 0 \tag{11}$$

With solution of the form,

$$E(\omega) = A^{+}e^{i(k^{+}.r-\omega t)} + A^{-}e^{i(k^{-}.r-\omega t)}$$
(12)

where A^+ and A^- are the amplitude intensity of the forward and backward electric field and the resultant cavity dispersion is obtained as

$$k_y^2 + k_z^2 = \frac{\omega^2}{c^2} \varepsilon(\omega) \tag{13}$$

Here k_y and k_z are the components of electric fields wave vectors along the plane and growth directions of the quantum well respectively.

Next, the dispersion relation of the quasi-particles materials is determined considering the incident angle depicted in Fig, 1 above. The cavity length L_c defined by cavity resonance frequency $\omega_c = \frac{\pi c}{l_c \sqrt{\varepsilon_b}}$ and mapping Equation (11) and Equation (13), we finally

arrived at:

$$\theta = \sqrt{\frac{\varepsilon_b}{\varepsilon_{cap}}} \left(1 - 4\pi Re\{\chi(\omega)//\varepsilon_b\} - \frac{\omega_c}{\omega^2} \right) \quad (14)$$

RESULTS AND DISCUSSION

The main parameters extracted from adjusting the exact Nonequilibrium results to the simple Lorentzian formula of Equation. 1 are summarized in Table 1, together with details of the cavity.



Figure 3: Imaginary part of optical susceptibility for transition between fist three subbands as used as the fitting parameters in the dielectric formalism of the palariton problem

The numerical results below are for two samples with either 10nm or 5nm GaAs/Al_{0.3}Ga_{0.7}As QWs in the active layer. The cavity is composed of 170 QWs, the lower barrier width $L_b = 150$ nm and top barrier $L_{b2} = 250$ nm to complete the sample for the required cavity length. The top and lower AlAs layers have 1300 nm each in both cases.

Table 1: Parameters used in the simulations delivered in Figs. 2. and 3. for increasing carrier density ΔN . μ , $\nu = 1,2$ denote, respectively the first and second subbands. $\Lambda_{\mu\nu}$ and $\omega_{\mu\nu}$ are obtained by adjusting the full numerical many body expression to the Lorentzian approximation in Eq. 1

<u>10nm</u>			5nm		
$L_{c} = 28.5 \mu m;$	$\omega_{c} = 6.8568 \text{meV};$	<i>λ</i> = 0.0596;	$L_{c} = 26.6 \mu m;$	$\omega_c = 7.3579 \text{meV}$; <i>λ</i> =0.0319;
	$\varepsilon_b = 10.0392$			$\varepsilon_{b} = 10.0117$	
$\Delta N (cm^{-2})$	$\Lambda_{\mu\nu}$ (meV)	^ω μν(meV)	ΔN (cm ⁻²)	Λ(meV)	$\omega_{\mu\nu}$ (meV)
0.1×10^{12}	0.5350	10.0125	0.1×10^{12}	0.6392	21.5269
0.2×10^{12}	1.0023	10.2628	0.2×10^{12}	1.2440	21.7722
1.0×10^{12}	3.6739	11.7647	0.5×10^{12}	2.7879	22.7747
2.0×10^{12}	6.5709	13.5168	1.0×10^{12}	5.0651	24.2803

In Fig. 4. we show the influence of dephasing and the effect of changing the carrier densities for THz



Figure 4: THz intervalence band polaritons due to coupling of TE polarized cavity mode and intervalence band excitations for a 10nm MQWs. (a)-(d) for different population densities ΔN as indicated in Table 1. The polariton character is maintained even at high value of dephasing with high doping concentrations as can be seen in (d)

CONCLUSION

On conclusion, we investigated the interaction of TE Mode THz radiation and intervalence bands excitation delivering THz intervalence band polaritons. This is based on the model quantum well structure presented I the literature. The approach can improve the quantum efficiency of THz based devices in the strong coupling regime of THz radiations and intervalence bands transitions in GaAs/Al_{0.3}Ga_{0.7}As quantum wells. A Nonequilibrium many body approach for the optical response beyond the Hartree-Fock approximation is used as input to the effective dielectric function formalism for the polariton problem. The energy dispersions relations

in the THz range are obtained by adjusting the full numerical solutions to simple analytical expressions to improve clarity, allowing a broad audience to investigate similar phenomena. The method allows to combine predictive microscopic optical response calculations with a simple dielectric model for the cavity leading to a powerful design tool for THz Polaritonics.

intervalence band polaritons from for the sample with the

geometric structure shown in Fig. 1.

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