Modelling of Exciton-Polaritons

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ABSTRACT

To study the generation of exciton polaritons in a quantum well embedded in a semiconductor Fabry-Pérot microcavity with distributed Brag reflectors, a simple semi-classical auxiliary differential equation based model is proposed. The solutions are obtained using FDTD method considering only the excitations from ground to next excited states and one single QW resonance. The simulations are presented for GaAs quantum well in Al_{0.1}Ga_{0.9}As microcavity and a ZnS quantum well embedded in CdSe microcavity with 12 DBR layers on either side. Model is proved to be stable and agrees with properties of polarization associated with polariton dispersion. Results show that GaAs is a better quantum well material to generate polaritons than CdSe.

Keywords: Exciton-polaritons, quantum well, microcavity, distributed Bragg reflectors, GaAs, AlGaAs/AlAs, CdSe/ZnS

1. INTRODUCTION

An exciton is an excited electron-hole pair, strongly couple by coulombs forces forming a temporary dipole in conductance and valence bands of a semiconductor. In 1958, Hopfield [1] theoretically suggested the existence of a possible coupled state of an exciton as well as photon and gave the name polariton due to its strong polarization field. This was independently theorized by Agranovich [2]. Later, Hopfield [3] suggested that the exciton was only one kind of polariton and calculated the polariton fields under resonant conditions. The properties of the coupling of an exciton and photon give a mixed set of properties of both
exciton and photon. One such property is its effective mass which is smaller than the electronic rest mass as it is combined with its massless photonic counterpart. Hence, these are very promising in applications in optoelectronics.

The optical properties of quantum wells (QW’s) can be significantly altered by embedding of the QW’s in dielectric structures such as a microcavity. After the pioneering studies by Weisbuch and coworkers [4, 5], interest in semiconductor microcavities embedded quantum wells (QW’s) increased due to microcavities having potential applications in the development of low-threshold vertically emitting lasers and also due to the fundamental aspects of the interaction of confined photon modes with matter opening a new field in quantum electrodynamics. The simplest semiconductor microcavity structure is a planar Fabry-Pérot cavity, bounded by dielectric mirrors called distributed Bragg reflectors (DBRs) forcing photons to bounce back. One of the main methods of creating exciton-polaritons is the use of a Febry-Perot mode cavity in which light of a specific wavelength is reflected in order to excite the electrons in the given semiconductor continuously [5]. A DBR is made of several identical pairs of two \( \lambda / 4 \) dielectric layers. For a large number of pairs \( (N) \), a DBR has a frequency region known as stop band in which the reflectivity is close to unity, whose centre is determined by the \( \lambda / 4 \) condition and width proportional to the difference of refractive index of the two constituents. The resulting structure is a solid state monolithic Fabry-Pérot cavity [6]. When the microcavity contains in a QW, the emission from the confined electronic states is strongly modified by the presence of the cavity. In general, two kinds of recombination processes can occur in semiconductors. The electron-hole recombination, which has a broadband, dipole-like emission pattern and excitonic emission having a very narrow line width, and whose emission pattern is subject to crystal momentum conservation rule. In confined systems like QWs, breakdown of crystal-momentum conservation along the growth direction leads to an intrinsic radiative lifetime of free excitons with an in-plane wave vector smaller than the wavevector of light [7]. When the in-plane coherence length of the exciton centre-of-mass motion is large, the emission is highly directional, and very different from dipole-like emission.

Chen, et al. [8] introduced a model to study the dynamic properties of the exciton-polariton based solely on the original equations derived by Hopfield [3]. Another model was developed by Zeng, et al [9] to model the polariton resonance variations with the electric field in time within quantum well structures. However, all these models used a microcavity or quantum well which is either infinite in nature or constrained to a Bohr radius thick spherical cavity. Hellstrom [10] used the Lorentz oscillatory model to simulate the polariton without incorporating any of the extra fields mentioned in the model proposed by Hopfield. Different theoretical schemes have been proposed to describe the exciton cavity system ranging from a semi-classical linear-dispersion model, in which the active medium is represented by a Lorentz oscillator [11-13] to a full quantum theory of the exciton-photon interaction in which the complex mixed-mode energies are derived from the poles of the Green function [6, 14-15].

In this paper to study the exciton-polaritons on a quantum well with a single atom thick radius at the centre of a Fabry-Pérot microcavity of finite thickness with distributed Bragg reflectors (DBR), a model based on semi-classical theory is proposed. The polarization dispersion are calculated and the numerical solutions are obtained using 2-dimensional FDTD analysis. The simulations are presented for GaAs quantum well sandwiched between two layers of \( \text{Al}_{0.1}\text{Ga}_{0.9}\text{As} \) microcavity on either side and 12 \( \text{Al}_{0.3}\text{Ga}_{0.7}\text{As} \) and \( \text{AlAs} \) DBR layers on
either side of the microcavity. The same model is used to study polariton resonance on II-VI materials namely, on a ZnS quantum well on a CdSe microcavity with DBR layers on either side. Only excitations from ground to next excited state (valance to conduction band) were assumed and one single quantum well resonance was considered.

2. METHOD

When an electron in the valence band of a semiconductor is excited to the conduction band, a hole is formed at the valence band and a Coulomb force exists between the conduction band electron and the valence band hole. Due to this interaction, the total energy between the electron and hole reduces by an amount $E_x \phi$ from the bottom of the conduction band which is known as exciton binding energy. The lifetime of an exciton is in the order of nanoseconds and hence the conduction band electron comes back to the valence band emitting a photon. If the energy of the photon ($E_{\text{photon}}$) is exactly equal to the energy gap ($E_g$) plus the reduce amount ($E_x \phi$), then a resonant exciton is created or if $E_{\text{photon}} < E_g + E_x \phi$, a general exciton is formed as shown in Fig. 1. In order to describe the change in electron and hole velocities in the lattice due to strong influence of the periodic atomic potentials, the concept of effective mass inside a particular semiconductor material is used. The reduce energy ($E_x \phi$) is a negative energy and can be given by the effective mass of the electron ($m_e^*$) and the hole ($m_h^*$):

$$E_x \phi = -\frac{e^4}{32 \pi^2 \hbar^2 \varepsilon_s^2 \varepsilon_0^2} \left( \frac{1}{m_e^*} + \frac{1}{m_h^*} \right)$$  \hspace{1cm} (1)

In traditional semiconductors made of inorganic materials, photo-excited electrons and their holes behave for most intents and purposes, as separate particles. In these weakly bound exciton states, called Wannier or Wannier-Mott excitons, the electron-hole pair is not tightly bound and the particles can be thought of being separated by many inter atomic spacing. Hence the properties of the Wannier-Mott exciton can be calculated using an effective mass approximation.

The electron and the hole can be thus considered as two moving particles but separated by many lattice distances within this approximation. Unlike atoms, the excitons have a finite life-time and the effective mass approximation allows neglecting, the periodic crystal potential and describes electrons and holes as free particles having a parabolic dispersion. The mass of the exciton $M$ can be perceived as their sum:
$$M = m_e^* + m_h^*$$  \hspace{1cm} (2)

The Wannier-Mott exciton can be compared to a positronium, an electron-positron pair. Also, the attractive Coulomb force is reduced by the dielectric constant $\varepsilon$ of the intervening medium.

A semiconductor microcavity of width $\lambda/2$ is shown in figure 2. The refractive index of the quantum well is $n_{QW}$ and the embedded cavity of refractive index $n_C$ is constructed to trap exciton-polaritons using a Fabry-Perot type two Bragg reflectors of width $\lambda/4$ kept on either side to reflect light within its distance. The DBR consists of the same two alternating layers with refractive indices $n_1$ and $n_2$, one higher than the other causing light reflecting from either side to destructively interfere, creating the stop band for transmission. Hence any light which entering the cavity with a wavelength close to the wavelength of the stop band or a multiple of the same wavelength will keep on reflecting inside. This phenomenon is called cavity resonance. If $\lambda_c$ is the cavity wavelength, then cavity width of $\lambda_c/2$ will trigger the resonance state. The refractive index of air is $n_0$.

A semiconductor QW is a thin layer of semiconductor with a thickness in the range of the de Broglie wavelength sandwiched between two layers of two semiconductors in contact, creating a potential barrier due to energy difference of the valence and the conduction bands. This variation in the bandgaps creates the quantum well confining the electrons to the specific semiconductor [16, 17]. 2D structures possess confinement of motion in one spatial direction.

The energy confinement ($E_{con}$) of the electron from Heisenberg’s uncertainty principle can be written as:

$$E_{con} = \frac{(\Delta p_x)^2}{2m_e^*} \sim \frac{\hbar^2}{2m_e^*(\Delta x)^2}$$

If $E_{con} < 1/4k_B T$, then $\Delta x = \hbar(8m_e^*k_BT)^{-1/2} \sim \lambda_{deB}$. This is the maximum length a quantum well could take to keep its properties intact.
When a quantum well is formed in semiconductors, as shown in Fig. 3 energy gap of the cavity \(E_{gc}\) is given by the difference in the energies between conduction and valence band and the energy gap of the quantum well \(E_{gqw}\) is given by the mid layer energy gap. Due to the nuclear mass being much larger than the electron mass this can be easily assumed. The semiconductor quantum well is confined to two free dimensions (x and y). If we consider a photon to move only in one direction perpendicular to y axis in x direction and if all layers are normal to the direction of the photons, then all effects in 3-dimensional space can be ignored in z direction and the model becomes a 2-dimensional model.

Therefore, the model uses 3-dimentional equations for quantum wells in 2-dimensional space.

Since nonlocal semi-classical theory and full quantum theory give equivalent descriptions for describing the optical properties of excitons in a planar and symmetric semiconductor microcavity [18], the semi-classical theory will be used. The semi-classical theory is clearly the most appropriate one to compute reflectivity \(R\), transmission \(T\), and absorption [6]. The exciton-radiation interaction in QW is based on a nonlocal susceptibility treatment of the optical response within the QW [7]. The nonlocal susceptibility is calculated in linear response theory, with nonresonant energy denominators neglected. The pioneering work of Hopfield [1], lead to the understanding that the coupling of excitons and photons can be summed up by the Maxwell’s electromagnetic equations with a strong polarization factor. Concepts such as the Lorentz model for harmonic oscillators help in understanding the variation of polarization and its importance in modelling polaritons. As the frequency of the electromagnetic radiation increases and approaches the characteristic vibrational frequencies associated with the lattice, strong interactions can occur modifying the dielectric function substantially. The interactions may be described quite successfully, by treating the solid to be a collection of damped harmonic oscillators, with a characteristic vibrational frequency or resonance frequency \(\omega_0\). Since the nucleus of the atom is much more massive than the electron, the atom in the Lorentz model is assumed to an electron-spring system connected to an infinite mass not movable.

The assumption that the binding force behaves like a spring is a justified approximation for any kind of binding, given that the displacement is small enough. The damping term comes from internal collisions and radiation emitted. The forces acting on the electron can be summed up as the Coulomb’s force acing on the electron \(F_d\), the force due to oscillation \(F_0\) with \(k\) being the spring constant and the damping force \(F_0\) opposing the motion:
\[ F = F_d - F_r - F_0 \Rightarrow m_e \ddot{r} = -eE - kr - \Gamma \nu \Rightarrow m_e \ddot{r} + eE + kr + \Gamma \nu = 0 \] (4)

where \( e \) is the electronic charge, \( r \) is the displace distance from equilibrium \( \nu \) is the velocity of electron and \( \Gamma \) is the damping factor.

**Fig. 3.** Forces acting on an electron in the Lorentz model

Given that the plasma frequency of the material, \( \omega_p = (ne^2/\varepsilon_0 m_e)^{1/2} \), the dielectric constant has the form [19]:

\[ \frac{\varepsilon}{\varepsilon_0} = 1 + \frac{\omega_p^2}{\omega_0^2 - \omega^2 + i\Gamma \omega} \] (5)

and the electric polarization vector \( P \):

\[ P = \varepsilon_0 \left( \frac{\varepsilon}{\varepsilon_0} - 1 \right) E = \frac{\omega_p^2}{\omega_0^2 - \omega^2 + i\Gamma \omega} E \] (6)

Exciton-polaritons are particles coupled with light. While the Lorentz model captures the essence of this, to show the action of the polariton an additional term was introduced to the polarization \( P \) by Hopfield [3] and later improved by many others [20, 21]:

\[ P = \frac{4\pi \beta_0 \omega_0^2}{\omega_0^2 - \omega^2 + \hbar \omega / M^*} \omega_0 - i\Gamma \omega} E \] (7)

where the oscillator strength \( \beta_0 = 2D^2 / \hbar \omega \) is given by the matrix element of exciton dipole interaction \( D \) and resonant frequency of exciton \( \omega_0 \) and \( M^* \) is the total effective mass of exciton given in equation 2.
Because excitons in a macroscopic system spread through the whole structure with an appropriate dispersion, they must be treated with a nonlocal theory [22]. Linear response theory constitutes such a theory, giving the dielectric polarization within a quantum well (QW) as:

\[ P(x, \omega) = T(\omega) \psi(x) \int \psi(x') E(x', \omega) dx' \]  

where \( \psi(x) = \psi(r, r) \) is the ground state wave function of the exciton excited in the QW microcavity and is given by [23]:

\[ \psi(r, r_b) = \frac{1}{|r - a| \sqrt{2\pi d_{cov}}} \sin \left( \frac{\pi |r - a|}{R} \right) \frac{1}{\sqrt{\pi a_B^3}} e^{(r - r_b)/a_B} \]  

\( a \) is the centre of quantum well and \( T(\omega) \) is the coefficient given by:

\[ T(\omega) = \frac{2 \pi \varepsilon_0 \varepsilon_b \omega_{LT} \omega_0 a_B^3}{\omega_0^2 - \omega^2 - 2i \Gamma \omega} \]  

where \( a_B \) is the Bohr’s radius in the corresponding bulk semiconductor, \( \varepsilon_b \) is the dielectric index of the well material and \( \omega_{LT} \) is the longitudinal-transverse splitting. \( \beta_0 = \varepsilon_0 \varepsilon_b \omega_{LT} \omega_0 / 2 \) forms the Lorentz model.

This can be summarized as:

\[ \hat{E}(x, \omega) = \sin \left( \frac{\pi |x - a|}{d_{QW}} \right) \int \left( \frac{\pi |x - a|}{d_{QW}} \right) E(x, \omega) \frac{dr}{d_{QW}^3} \]  

Hence it is possible to rewrite equation 7 as:

\[ P = \frac{4 \pi \beta_0 \omega_0^2}{\omega_0^2 - \omega^2 + \frac{\hbar k^2}{M^*} \omega_0 - i \Gamma \omega} \hat{E}(x, \omega) \]  

\( \omega_0 \) is the ground-state exciton resonance frequency. Within the quantum well, the dielectric constant drastically changes, affecting the photons entering the quantum well. Exciton dispersion occurs at ground state when \( \omega_0 = \omega \).

Similarly, a photon has a frequency given by \( \omega = k_0 c \) where \( k_0 \) is the wave number of light in free space. The strong coupling of these two gives rise to the polariton in question and therefore the polarization field plays a vital role in observing the coupled effects.
3. FDTD ANALYSIS OF THE MODEL

An exciton polariton is essentially a travelling electromagnetic wave coupled with an electron. Hence a polariton can be modelled using finite difference time domain (FDTD) analysis. Electric fields are normalized so that the $E$-field and the $H$-field have the same order of magnitude and the normalized Maxwell’s equations read

$$\nabla \times E = -\left[ \frac{\mu_r}{c} \right] \frac{\partial B}{\partial t}; \quad \nabla \times H = \left[ \frac{\varepsilon_r}{c} \right] \frac{\partial D}{\partial t}$$

where $D(t) = \varepsilon_r \varepsilon_0 (E(t) + 4\pi P(t))$; $B(t) = \mu_r \mu_0 H(t)$, $c$ is the speed of light in vacuum. Assuming the tensors $[\mu_r]$ and $[\varepsilon_r]$ exists along the diagonal only, the above equations can be expanded as:

$$\frac{\partial E_k}{\partial x_j} - \frac{\partial E_j}{\partial x_k} = -\frac{1}{c} \left( \mu_{ij} \frac{\partial H_j}{\partial t} \right); \quad \frac{\partial H_k}{\partial x_j} - \frac{\partial H_j}{\partial x_k} = \frac{1}{c} \left( \varepsilon_{ij} \frac{\partial D_j}{\partial t} \right) \quad (13)$$

$$D_i(t) = \varepsilon_{ii} (E_i(t) + 4\pi P_i(t))$$

The finite difference equations can be written under the Yee Grid developed by Yee [24]. Adopting the Yee Grid is important as by design it gives the curl of electric field $E$ at the centre of the grid in transverse electric (TE) mode and the curl of magnetic field $B$ (or $H$ since $B=H$) at the centre of the grid in transverse magnetic (TM) mode. The model used in this dissertation is in 2-dimensional space hence $\Delta z = 0$ and also must be noted that each step of magnetic field component lies a half a time step in front. Therefore equations 13 has the form:

![Diagram of Yee Grid](Diagram.png)  

5(a)
Fig. 5. (a) Yee grid - Locations and orientations of electric and magnetic fields per cell defined such that Maxwell’s equations are satisfied, (b) 2-dimensional TE mode (left) and TM mode (right) of the unit Yee grid cell.

\[
\frac{E_{z}^{i+1,j,k} - E_{z}^{i,j,k}}{\Delta y} = -\frac{\mu}{c} \left( H_{x}^{i,j,k} \big|_{r=\Delta r/2} - H_{x}^{i,j,k} \big|_{r=-\Delta r/2} \right); \quad \frac{E_{x}^{i+1,j,k} - E_{x}^{i,j,k}}{\Delta x} = \frac{\mu}{c} \left( H_{y}^{i,j,k} \big|_{r=\Delta r/2} - H_{y}^{i,j,k} \big|_{r=-\Delta r/2} \right)
\]

\[
\frac{E_{y}^{i+1,j,k} - E_{y}^{i,j,k}}{\Delta x} - \frac{E_{y}^{i,j+1,k} - E_{y}^{i,j,k}}{\Delta y} = -\frac{\mu}{c} \left( H_{z}^{i,j,k} \big|_{r=\Delta r/2} - H_{z}^{i,j,k} \big|_{r=-\Delta r/2} \right)
\]

\[
\frac{H_{z}^{i,j,k} \big|_{r=\Delta r/2} - H_{z}^{i,j,k} \big|_{r=-\Delta r/2}}{\Delta y} - \frac{H_{y}^{i+1,j,k} - H_{y}^{i,j,k}}{\Delta x} = -\frac{\varepsilon}{c} \left( E_{x}^{i,j,k} \big|_{r=\Delta r/2} - E_{x}^{i,j,k} \big|_{r=-\Delta r/2} \right)
\]

\[
\frac{H_{y}^{i,j,k} \big|_{r=\Delta r/2} - H_{y}^{i,j,k} \big|_{r=-\Delta r/2}}{\Delta x} - \frac{H_{x}^{i,j+1,k} - H_{x}^{i,j,k}}{\Delta y} = -\frac{\varepsilon}{c} \left( E_{x}^{i,j,k} \big|_{r=\Delta r/2} - E_{x}^{i,j,k} \big|_{r=-\Delta r/2} \right)
\]

The polarized electric field coupled with the electrons in the microcavity \( \hat{E} \):

\[
\hat{E}_{i} = \frac{1}{\varepsilon} (D_{i} + 4\pi P_{i})
\]

The \( 4\pi \) in eq.15 has already been added in the polarization in the Lorentz model given by eq. 11 hence it can be omitted in the calculations.

Light used in this simulation is unpolarised and has a wide range of frequencies. Hence to simulate the unpolarised light source which is not coupled with the microcavity electrons, the electric field uncoupled and moving freely within the system is \( E \):

\[
D(t) = \varepsilon_{0}\varepsilon E(t)
\]
Eq. 12 can be written as:

\[
\left(\omega_0^2 - \omega^2 + \frac{\hbar k^2}{M^*} \omega_0 - i\Gamma \omega\right) \mathbf{P}(\omega) = 4\pi\beta_0 \omega_0^2 \hat{\mathbf{E}}(\omega)
\]

Using Fourier transform, the polarization and electric field can be changed to time domain:

\[
\mathbf{P}(t) = \frac{1}{2\pi} \int \mathbf{P}(\omega)e^{-i\omega t} d\omega; \quad \hat{\mathbf{E}}(t) = \frac{1}{2\pi} \int \hat{\mathbf{E}}(\omega)e^{-i\omega t} d\omega
\]

\[
\left(\omega_0^2 + \frac{\hbar k^2}{M^*} \omega_0\right) \mathbf{P}(t) + \frac{\partial^2}{\partial t^2} \mathbf{P}(t) + \Gamma \frac{\partial}{\partial t} \mathbf{P}(t) = 4\pi\beta_0 \omega_0^2 \hat{\mathbf{E}}(t)
\]

Introducing a new term \( \mathbf{J} = \frac{\partial \mathbf{P}}{\partial t} \), the above equation read:

\[
\frac{\partial}{\partial t} \mathbf{J}(t) + \Gamma \mathbf{J}(t) + \left(\omega_0^2 + \frac{\hbar k^2}{M^*} \omega_0\right) \mathbf{P}(t) = 4\pi\beta_0 \omega_0^2 \hat{\mathbf{E}}(t)
\]  

(17)

Eq. 17 on the Yee grid:

\[
(2 + \Gamma \Delta t) \mathbf{J}^{t+\Delta t/2} - (2 - \Gamma \Delta t) \mathbf{J}^{t-\Delta t/2} + 2\Delta t \left(\omega_0^2 + \frac{\hbar k^2}{M^*} \omega_0\right) \mathbf{P}^t = 4\pi\beta_0 \omega_0^2 \hat{\mathbf{E}}^t
\]  

(18)

From the definition of \( \mathbf{J} \), polarization:

\[
\mathbf{P}^t = \mathbf{P}^{t-\Delta t} + \Delta t \mathbf{J}^{t-\Delta t/2}
\]  

(19)

For the simulation, a method is needed to terminate the wave or make it appear to go up to infinity without reflecting at the boundaries. As it stands, there is a total reflection at the boundary and this is overcome by using what is known as a perfectly matched layer (PML).

A PML essentially is an absorbing layer which diminishes the wave completely. In this simulation a uniaxial perfectly matched layer (UPML) technique of Zachary, et al [25] is incorporated on the top and bottom as shown in Fig. 6.

Total-field/scattered-field (TF/SF) boundary separates the transmitted beam from the scattered beam in contact with the device while the UPML on either side absorbs the scattered fields.

Further the update equations are fixed on the left and right side by making them periodic (periodic boundary conditions) in nature which means whatever leaves the grid from either one of those sides will appear on the other side entering the grid.
Fig. 6. The periodic boundaries prevent any scattered signal leaving these boundaries by re-injecting the fields from the opposing side.

All simulations were carried out on MATLAB R2013b software and all codes were written in order to enhance the polariton formation. However, in order to generate the main visualization of the fields, a function created by CEM labs was used (Rumpf, 2012). This function is used to show visually the superimposed fields propagating through an entire grid in an FDTD simulation.

For the simulations a Gaussian source was used with the basic form:

\[ E_{\text{source}} = e^{-(t-t_0)^2/\tau^2}; \quad H_{\text{source}} = \frac{E_0}{\sqrt{\mu_0}} e^{-(t-t_0+\delta t)^2/\tau^2} \]  

(20)

where \( t \) is the number of time steps, \( \tau \) is the time variance around central frequency \( f_0 \), \( t_0 \) is the mean time (\( t_0 = 10/f_0 \)) and \( \delta t \) is the phase shift. In order to test the central cavity, a simulation was done without the DBR on either side. The central cavity is expected to show an increased transmittance at the specific frequency given by:

\[ n_{\text{cav}} = \frac{\lambda_0}{d_{\text{cav}}} \]  

(21)

where \( n_{\text{cav}} \) is the refractive index of the cavity and \( d_{\text{cav}} \) is the length of the cavity. The wavelength \( \lambda_0 \) for the energy 1.518 eV:

\[ \lambda_0 = \frac{2\pi hc}{1.518} = 817.1\text{nm} \]  

(22)

In modelling the central cavity, \( E \) as well as \( \hat{E} \) were simulated simultaneously. It is expected that there would be a high transmittance at 1.518 eV as \( d_{\text{cav}} = 67.5 \text{nm} \) and \( n_{\text{cav}} = 12.1 \). The stop band frequency bandwidth \( \Delta f \) for the central frequency \( f_0 \) is given by:
\[
\frac{\Delta f}{f_0} = \frac{4}{\pi} \sin^{-1}\left(\frac{n_2-n_1}{n_2+n_1}\right)
\]

Intensity of the polarization field \( I_{pz}(x,y,t) \) is calculated by:

\[
I_{pz}(x,y,t) = \sqrt{P_z(x,y,t) \times P_z^*(x,y,t)}
\]

where \( P_z \) is the polarization value at point \( x, y \) at time \( t \) and \( P_z^* \) is the conjugate polarization value at point \( x, y \) at time \( t \). The drop in electric field intensity \( I_{ez}(x,y,t) \) due to the polariton at that point:

\[
I_{ez}(x,y,t) = \frac{1}{\varepsilon_0 c(x,y)} I_{pz}(x,y,t)
\]

Note that both \( I_{ez} \) and \( I_{pz} \) are quantities similar to the polarization and electric field components in and surrounding the quantum well.

The properties of the polaritons created on the semiconductor used, is entirely dependent on the polarization equation. Hence by isolating the polarisation field given by eq. 7 to the central cavity within the quantum well implanted, the polariton can be modelled. Here it is assumed that the quantum well is one or few atoms thick and is infinite in y direction. Furthermore, the effect of eq. 8 is used here to isolate the polariton within this well.

Transmittance \( (T) \) is given by:

\[
T = \left[1 - \left(\frac{n_0(n_z)^{2N} - n_{sub}(n_1)^{2N}}{n_0(n_z)^{2N} + n_{sub}(n_1)^{2N}}\right)^2\right]
\]

where refractive index of the originating medium is \( n_0 \) and the substrate is \( n_{sub} \) and the number of repeated pairs of layers is \( N \).

4. POLARITON RESONANCES IN III-V MATERIALS

![Fig. 7. Ez at 150 time step out of 25218 for a DBR of 24 pairs of layers using FDTD Simulation](image-url)
Polariton resonances in a GaAs quantum well embedded in a Al$_{0.1}$Ga$_{0.9}$As microcavity was studied and simulated. A simulation for 24 pairs of Al$_{0.3}$Ga$_{0.7}$As and AlAs DBR layers with refractive indices 3.4205 ($n_1$) and 3.1305 ($n_2$) respectively in x-y direction using FDTD method is presented in fig 7. Light coloured layer has a refractive index of $n_1$ and the dark coloured layer has a refractive index of $n_2$. Both layers have lengths $L_1 = \lambda_0/4n_1$ and $L_2 = \lambda_0/4n_2$ respectively. An 1.518 eV energy yield a stop band transmittance of 0.081% and a bandwidth of 0.1127 eV.

In order to find the DBR layer facing the inner part of the microcavity, transmittance for different photonic energies were tested for $n_1 > n_2$ and $n_2 > n_1$.

These are shown in fig. 8(a) and 8(b) respectively. When $n_1 > n_2$, the centre frequency or photonic energy is at 1.56 MeV around which the stop band was made. The correct value of 0.08% transmittance and 0.1 eV bandwidth was observed. For $n_2 > n_1$, although the centre frequency or photonic energy showed at 1.56 eV around which the stop band, an anomalous area exists in the stop band in which the stop band has a higher transmittance than calculated. However, the bandwidth remains close to the value calculated.

Modelling the central cavity with $n_{cav} = 3.4785$ and $d_{cav} = 234.9$ nm, the electric fields $E$ as well as and polarized electric fields $\hat{E}$ were simulated simultaneously for polariton resonances in a Al$_{0.1}$Ga$_{0.9}$As microcavity embedded in GaAs quantum well surrounded by 24 set of DBR mirrors.
The parameters used for the simulations are presented in Table 1. Here it is assumed that the quantum well is one or few atoms thick and is infinite in y direction.

The $z$-components of dispersion of electromagnetic wave ($E_z$) in a GaAs quantum well and its polarized component ($\hat{E}_z$) creating polaritons in a DBR microcavity at 540, 1300, 2130 and 13650 time steps out of 16115 in $x$ and $y$ directions are presented in fig. 9(a)-9(d). Due to the formation of polaritons within the cavity, the polarized electric field centres itself in the range of the microcavity.

**Table 1.** Parameters used to simulate the Al$_{0.1}$Ga$_{0.9}$As microcavity in GaAs quantum well

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exciton Energy ($\hbar \omega$)</td>
<td>1.518 eV</td>
</tr>
<tr>
<td>Exciton broadening parameter ($\Gamma$)</td>
<td>0.1 meV</td>
</tr>
<tr>
<td>Exciton effective mass ($M^*$)</td>
<td>0.49 $m_0$</td>
</tr>
<tr>
<td>Exciton oscillator strength ($4\pi\beta$)</td>
<td>$1.325 \times 10^{-3}$</td>
</tr>
<tr>
<td>Al$<em>{0.1}$Ga$</em>{0.9}$As dielectric constant ($\varepsilon_{ow}$)</td>
<td>12.1</td>
</tr>
<tr>
<td>GaAs dielectric constant ($\varepsilon_{QW}$)</td>
<td>12.53</td>
</tr>
</tbody>
</table>

**Fig. 9.** Dispersion of electromagnetic wave (above) in a GaAs quantum well and its polarized component (bellow) creating polaritons in a DBR microcavity at (a) 540, (b) 1300, (c) 2130 and (d) 13650 time steps out of 16115.

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The electric polarization intensity in the system for the TM mode with distance and the transmittance percentage of photons at different energies are shown in fig. 10(a) and 10(b) respectively. A high polarization field at the centre of the quantum well as well as a high transmission is observed at the relevant photon energy at which the exciton is formed.

A more controlled analysis can be obtained when the system is under stable conditions. The polarized electric field intensity for different GaAs quantum well widths (0-300 nm), oscillator strengths and effective mass ratio $M^*/m_0$ in log scale for the system with DBR mirrors are presented in fig. 11(a), 11(b) and 11(c) respectively. In order to get good polaritons, the electric polarization value should be maximized. The polarization and quantum well width shows an exponential relationship and therefore effects of the polariton decrease as the width increases. Below 10 nm energy conservation drops
drastically. The relationship between oscillator strength and the polarization value is linear. As the effective mass of the electron increases, the polariton model falls out of Lorentz oscillator form. But as the effective mass of the electron reaches a constant value, its value increases above the mass of an electron and therefore this model still satisfies the equations of the polariton.

5. POLARITON RESONANCES IN II-VI MATERIALS

The same model was used to simulate polariton resonances in ZnS microcavity embedded in CdSe quantum well. The electric fields $E$ as well as and polarized electric fields $\hat{E}$ were simulated simultaneously for polariton resonances in a ZnS microcavity embedded in CdSe quantum well surrounded by 24 set of DBR mirrors. The parameters used are tabulated in Table 2. The $z$-components of dispersion of electromagnetic wave ($E_z$) (above) in a CdSe quantum well and its polarized component ($\hat{E}_z$) (below) creating polaritons in a DBR microcavity at $(a)$ 490, $(b)$ 1210, $(c)$ 2390 and $(d)$ 12640 time steps out of 15238.

Table 2. Parameters used to simulate the ZnS microcavity in CdSe quantum well

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exciton Energy ($\hbar \omega$)</td>
<td>1.700 eV</td>
</tr>
<tr>
<td>Exciton effective mass ($M^*$)</td>
<td>0.13 $m_0$</td>
</tr>
<tr>
<td>Width of quantum well</td>
<td>100 nm</td>
</tr>
<tr>
<td>ZnS dielectric constant ($\varepsilon_{\text{ZnS}}$)</td>
<td>2.24</td>
</tr>
<tr>
<td>CdSe dielectric constant ($\varepsilon_{\text{CdSe}}$)</td>
<td>2.44</td>
</tr>
</tbody>
</table>

![Fig. 12. Dispersion of electromagnetic wave (above) in a CdSe quantum well and its polarized component (below) creating polaritons in a DBR microcavity at (a) 490, (b) 1210, (c) 2390 and (d) 12640 time steps out of 15238.](image)
polaritons in a DBR microcavity at 490, 1210, 2390 and 12640 time steps out of 15238 in x and y directions are presented in fig. 12(a)-12(d).

13(a) Electric polarization intensity with distance 13(b) Transmittance of photons with energy

Fig. 13. 13(a) Electric polarization intensity with distance. 13(b) Transmittance of photons with photon energy in the microcavity embedded at the centre of a quantum well surrounded by 12 DBR layers.

The electric polarization intensity with distance in the system and transmittance percentage of photons at different energies are shown in fig. 13(a) and 13(b) respectively. Transmission is seen around the 1.7 eV range. Once again there exists a sudden drop in conservation close to the exciton’s exciting energy. This may be the result of the polariton formation as in II-V case When the system is under stable conditions, the polarized electric field intensity for different CdSe quantum well width (0-300 nm), is presented in fig. 14.

The CdSe quantum well also follows the same pattern as a GaAs quantum well in terms of the relationship between the width of the quantum well and the Electric field intensity. However, the intensity value is slightly lower in CdSe well than that of GaAs. It is more likely that GaAs has a better rate of producing polaritons.
6. CONCLUSIONS

The model proposed here incorporates the most important equations needed to generate polaritons using a combination of the initial works in this field and the latter findings by others. This model has proved to be stable and agrees with properties of polarization associated with polariton dispersion. The most basic tests were performed to test the new proposed model such as to change different parameters and observe the variation in the polarization field. Many factors including effective mass, oscillation strength and quantum well length was compared and by simulation it was concluded that the highest polarization was observed when the oscillation strength is high (above 0.1) and length of the quantum well is as low as possible. Furthermore, as the effective mass increases, the polarization increases. Hence, higher the effective mass, higher is the strong coupling. GaAs has a higher effective mass than CdSe. By numerical comparison between GaAs and CdSe quantum wells simulated through this model it was found that GaAs quantum wells has a slightly higher electric field intensity compared to that of CdSe and hence it is likely that GaAs is a better quantum well to generate polaritons. From the visual representation of the exciton at the centre of the quantum well, the movement of photons can be seen as well as its interaction with the quantum structure.

References


