Electrorefraction in Quantum Dots.

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We developed a model to calculate the electrorefraction due to the Quantum Confined Stark Effect in strained cylindrical QDs. We followed a numerical matrix diagonalization method using an expansion in plane-wave states. The correct polarization dependence is obtained by using the 4X4 Luttinger-Kohn Hamiltonian for the valence band. The exciton wavefunction is also calculated using a diagonalization approach. We will present the absorption spectra as a function of applied electric field and dot dimensions and discuss the implications for the electrorefraction.

Introduction

Electro-absorption modulators and Mach-Zehnder Interferometric (MZI) space switches [1] have mainly been developed using bulk or quantum well materials. In bulk semiconductor materials, the length of the phase shifting section is usually 2-4 mm. We have recently shown that this length can be decreased down to 0.46 mm in quantum well material by combining carrier depletion and the Quantum Confined Stark Effect (QCSE) in an asymmetric MZI switch [2]. This result shows that reducing the dimensionality of the semiconductor structure, provides improved performance phase shifters. In this contribution, we will investigate the possibility of quantum dot (QD) material for providing electrorefraction in the phase shifter of an MZI.

The conceptual advantage of QDs is the discrete density of states, resulting in narrow absorption peaks which shift with the applied electric field due to the QCSE. Bandfilling will decrease the oscillator strength of the QD absorption peaks. When choosing the operating wavelength to coincide with the peak of such a discrete absorption peak, both the QCSE and bandfilling result in a quickly decreasing absorption strength, resulting in electro-absorption. On the other hand, when choosing the operating wavelength just outside the discrete absorption peak, a clear electro-refraction effect is expected. In this contribution, we will present a model to calculate the electro-absorption and electro-refraction in QD material. In particular we will investigate the influence of the QD size on the QCSE and exciton oscillator strength [3]. The final goal of this work is to identify the potential of QD material for realistic electro-absorption modulators, electro-refraction based MZI’s as well as for all-optical signal processing based on bandfilling.

Theoretical approach

In our model we treat cylindrical InAs quantum dots with radius R and height h within a GaAs matrix. We assume a parabolic conduction mass with effective mass $m^*$. For the valence band, we use the 4X4 Luttinger-Kohn Hamiltonian with respect to the \{\ket{3/2,+3/2}, \ket{3/2,-3/2}, \ket{3/2,+1/2}, \ket{3/2,-1/2}\} basis and allow for strain as well as for the QCSE by adding the interaction with the electric field $F$ [4]

$$H_e = \hbar^2 \nabla (\frac{1}{2m^*(x,y,z)}) \nabla + V_e(x,y,z) + a_\epsilon \epsilon_{xy}(x,y,z) + eFz$$
Ve(x,y,z) and Vh(x,y,z) are the electron and hole confinement potentials with depth V\textsubscript{e0} and V\textsubscript{h0}, respectively. The third term in the Hamiltonian represents the hydrostatic strain acting in the conduction and valence band. P, Q, R and C have their usual meaning [5].

P\pm = p_x(\gamma_1 \pm \gamma_2)p_x + p_y(\gamma_1 \pm \gamma_2)p_y + p_z(\gamma_1 \mp 2\gamma_2)p_z

Q_z = 2\sqrt{3}\left[(p_x \pm ip_y)(\sigma - \delta)p_z + p_x \pi (p_x \pi (p_x \pm ip_y))\right]

R = \sqrt{3}\left[(p_x + ip_y)\mu (p_x + ip_y) - (p_x - ip_y)\gamma (p_x \pm ip_y)\right]

C = 2p_x(\sigma - \delta - \pi)(p_x - ip_y) - 2(p_x - ip_y)(\sigma - \delta - \pi)p_z

with \( \sigma - \delta = (-1 - \gamma_1 + 2\gamma_2 + 6\gamma_3)/6 \), \( \pi = (1 + \gamma_1 - 2\gamma_2)/6 \), \( \gamma = (\gamma_2 + \gamma_3)/2 \), \( \mu = -(\gamma_2 - \gamma_3)/2 \), in which \( \gamma_1(x,y,z) \), \( \gamma_2(x,y,z) \) and \( \gamma_3(x,y,z) \) are position dependent Luttinger effective mass parameters, representing the InAs and GaAs effective masses. To solve the envelope function equation we employ the numerical matrix-diagonalization scheme [6] by using single particle waves as expansion basis normalized in a cube with dimensions L\textsubscript{x}, L\textsubscript{y} and L\textsubscript{z}. The dimensionality of the Hamiltonian is chosen to ensure completeness within the Hilbert space, and for optimizing the computational time.

\[
\Psi_e(x_e,y_e,z_e) = \frac{1}{\sqrt{L_xL_yL_z}} \sum_{n,m,l} C_{e nml} e^{i(k_x+\frac{2\pi}{L_x}n)x_e+(k_y+\frac{2\pi}{L_y}m)y_e+(k_z+\frac{2\pi}{L_z}l)z_e}
\]

\[
\Psi_h(x_h,y_h,z_h) = \frac{1}{\sqrt{L_xL_yL_z}} \sum_{n,m,l} \begin{bmatrix} a_{nml} \\ b_{nml} \\ c_{nml} \\ d_{nml} \end{bmatrix} e^{i(k_x+\frac{2\pi}{L_x}n)x_h+(k_y+\frac{2\pi}{L_y}m)y_h+(k_z+\frac{2\pi}{L_z}l)z_h}
\]

where K\textsubscript{x}=2\pi/L\textsubscript{x}, K\textsubscript{y}=2\pi/L\textsubscript{y}, K\textsubscript{z}=2\pi/L\textsubscript{z} and n,m,l=0,±1, ±2, ±3,...

The optical properties of a quantum dot are strongly influenced by the exciton formation. The formation of the excitons will produce a red shift in the absorption spectrum with respect to the interband transition as well as enhanced oscillator strength. We describe the exciton states with the Hamiltonian
The Coulomb interaction term cannot be diagonalized in a single particle basis set. However, using the full set of solutions obtained for the electron and hole envelope wavefunctions $\Psi_e, \Psi_h$, we calculate the exciton wavefunction $\varphi_{\text{ex}} = \Psi_e \Psi_h$ by diagonalizing $< \varphi_{\text{ex}} | H_{\text{exc}} | \varphi_{\text{ex}} >$. Since the kinetic energy terms are functions of individual electron and hole coordinates, they are already diagonal to the single particle basis set. The confinement potential and the electric field will only shift the energy, without producing any band mixing and hence add to the diagonal terms. Hence, the only task is to diagonalize the Coulomb term with respect to the basis set of electron-hole product waves. The resulting excitonic confinement energy becomes $E_{\text{exc}} = E_e + E_h - E_b$, with $E_b$ the excitonic binding energy.

The absorption coefficient finally depends on the transition matrix elements and the exciton density $|\varphi_{\text{ex}}(0)|^2$. The full polarization dependence of the Bloch part of the transition matrix elements $< u_e \Psi_e | \epsilon \cdot p | u_h \Psi_h >$ is included following Yamanishi et.al [7,5] 

$$\alpha(h\omega) = \frac{\pi e^2}{n e \hbar c V} \frac{1}{\omega} \sum_i |\varphi_{\text{ex}}(0)|^2 \left| < u_e \Psi_e | \epsilon \cdot p | u_h \Psi_h > \right|^2 \Gamma(E_{\text{exc}} - h\omega)$$

where the transition matrix elements can be calculated either for TE or TM polarization, using the Luttinger-Kohn formalism. $\Gamma(E_{\text{exc}} - h\omega)$ is the homogeneous line broadening function, $n$ the bulk refractive index and $V$ the QD volume.

Figure 1: (Left) Quantum Confined Stark Effect in a cylindrical InAs/GaAs QD. It can be seen that the light-hole transition shows a larger red shift than the heavy-hole transition. For applications, electrorefraction due to the light-hole transition should thus be considered. (Right) Quantum dot absorption spectrum showing both the heavy-hole exciton absorption at 1.23 eV and the light-hole exciton absorption line at 1.35 eV for both TE and TM polarization.
Finally, the electro-refraction $\Delta n$ and the electro-absorption $\Delta \alpha$ are connected through the Kramers-Kronig relations

$$\Delta n = \frac{c}{\pi} P \int_{-\infty}^{\infty} \frac{\Delta \alpha}{(\omega')^2 - (\omega)^2} d\omega$$

**Quantum Confined Stark Effect in InAs-GaAs quantum dot**

In order to prove the reliability of the software we compare in Fig. 1 the QCSE in a InAs/GaAs quantum dot with 50Å radius and 30Å height with previous theoretical and experimental results [4], showing excellent agreement. From Fig.1 it is clear that the light hole (lh) transition energy will decrease sharply with increasing field strength. This is because the lh-state is close to the bulk GaAs valence band and hence the lh-wave function will leak more into the GaAs barrier, while the hh is more confined within the InAs dot. So the lh will experience a relatively large QCSE compared to the hh.

In Fig. 2, we finally present preliminary electrorefraction spectra of a single InAs/GaAs QD for both TE and TM polarization.

**Conclusions**

In conclusion, we present results for the electro-absorption and electro-refraction spectra of a single cylindrical InAs/GaAs quantum dot taking into account the 4x4 Luttinger Kohn Hamiltonian as well as strain. The model allows to calculate the exciton binding energy by a diagonalization technique. We find a larger QCSE red shift for the light-hole than for the heavy hole exciton transition.

**References**