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A THEORETICAL STUDY OF PHYSICAL PROPERTIES OF QUANTUM WIRE AND EVALUATION OF CHANGES OF REFRACTIVE INDEX AS A FUNCTION OF PHOTON ENERGY FOR DIFFERENT INCIDENT OPTICAL INTENSITIES AND FIXED LENGTH OF QUANTUM WIRE

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Abstract: - Using the theoretical formalism of Reza Khordad [J. Theor & Appl. Phys, 6, 19(2012)] and R Khordad etal [Commun. Theor Phys, 57, 1076(2012)], we have evaluated inter subband optical refractive index changes of the wire as a function of photon energy. The evaluation has been performed in two ways: (1) Keeping length of the wire fixed and varying the incident optical intensity (2) Keeping incident optical intensity fixed and varying the length of the wire. We observed that in the first case the total refractive index changes decreases with increase of the optical intensity. In the second case, the total refractive index changes decreases as the quantum size decreases. These results have great importance in the quantum confinement of the charge carriers of the nanostructured material. Our theoretically evaluated results are in good agreement with the other theoretical workers

Keywords: Quantum wire, quantum dots, Quantum confinement, Inter subband total refractive changes, Linear and nonlinear refractive index changes, Optoelectronic and photonic devices, Parallelogram Cross section.

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INTRODUCTION

In the past two decades, there has been considerable interest in the physics of low-dimensional semiconductor structures. These structures are superlattices, quantum wires, single and multiple quantum wells and quantum dots[1-8]. The physical properties of these structures have been extensively studied both theoretically and experimentally[1,2]. These structures confine charge carriers in one, two and three dimensions. Quantum confinement of the charge carriers in these structures leads to the formation of discrete energy levels, the enhancement of the density of states at specific energies. Due to these facts, the optical absorption spectra of the system are drastically changed. One of the most intensively explored classes of semiconductor structures is the class of quantum wires. With technological progress in the fabrication of semiconductor structures like chemical lithography, molecular beam epitaxy, and etcing, it has been made possible to fabricate a wide variety of quantum wires with well-controlled shape and composition. Among hetrostructures, quantum wires with rectangular, T-shaped, V-groove, triangular, and other cross sections have received lots of attention by researchers during the last decade[4-8].

The linear and nonlinear optical properties of low dimensional semiconductor structures are of considerable current interest in connection with their potential applications in optoelectronic and photonic devices[9,10]. It has been seen that there are many novel optical properties which are not seen in the bulk materials[11-13]. The linear and nonlinear optical properties of nanostructures have been widely studied by several workers[14,15]. The linear inter subband optical absorption within the conduction band of a GaAs quantum well without and with an electric field has been experimentally studied[16,17]. Nonlinear inter subband optical absorption in a semiconductor quantum well was also calculated by Ahn and Changin[18]. Rappen etal[19] studied the non-linear absorption for two-dimensional magnetoexcitons in $In_xGa_{1-x}As/In_yAl_{1-y}As$ quantum well. Bockelman and Bastard[20] discussed interband absorption in quantum wires with a magnetic field and without magnetic field[21]. Inter subband optical absorption in coupled quantum wells under an applied electric field was studied by Yuh and wang[22]. Cui etal[23] experimentally studied the absorption saturation of inte rsubband optical transitions in $GaAs/Al_xGa_{1-x}As$ multiple quantum wells. R Khordad[24] has studied the optical properties of quantum disk in the presence of an applied magnetic field. He has also investigated the optical properties of a modified Gaussian quantum Dot under hydrostatic pressure[25]. The inter subband optical absorption coefficients and refractive index changes in nanostructured materials have attracted considerable and continuous attention during one decade[26]. Wang etal[27] examined the refractive index changes induced by the incident optical intensity in a semiparabolic quantum well. Unlu etal[28] investigated the optical rectification in a semiparabolic quantum well. Several workers[29-32] have studied the optical properties of low-dimensional systems over last five to seven years.

In this paper, using theoretical formalism of Reza Khordad[33] and R. Khordad etal[34], we have theoretically studied the optical properties of quantum wire. We have evaluated inter subband refractive index changes as a function of photon energy for fixed value of incident optical intensity and length of the wire. We have performed three works related to optical properties of quantum wire. As a first work, we have evaluated linear, nonlinear and total refractive index changes for a given length of wire and incident optical intensity as a function of photon energy (meV). We observed that the linear refractive index change is opposite to that of nonlinear part. As a second work, we have determined the total refractive index changes keeping length of the wire fixed and varying the incident optical intensities. We observed that the total refractive index changes decreases as a function of photon energy with increase of the optical intensity. As a third work, we have calculated total refractive index changes as a function of photon energy keeping incident optical intensity fixed and varying the length of the wire. In this case, we observed that the total refractive index changes decreases as the quantum size L decreases. Our theoretically evaluated results are in good agreement with other theoretical workers[35-37].

MATERIALS AND METHODS:

Here, one solves the Schrodinger equation for an electron confined in a parallelogram quantum wire. One obtains the energy levels and wave functions analytically. Then, one tries to study the linear, nonlinear and total absorption coefficients and refractive index changes of the system. For this purpose, one considers only the two-level system for electronic transition. One shows that both the incident optical intensity and the structure parameter have great effects on the total absorption coefficients and refractive index changes of a parallelogram quantum wire.

The Hamiltonian of a charge carrier in a quantum wire is given by

$$H = -\frac{\hbar^2}{2m^*}\nabla^2 + V(x,y) \qquad (1)$$

Where m^* is the effective mass. V(x, y) is the confining potential

$$V(x, y) = 0, \quad \text{inside}$$
$$\infty, \quad \text{Outside} \qquad (2)$$

To obtain energy levels and wave functions, one solves the Schrodinger equation in the Cartesian coordinates

$$\frac{-\hbar^2}{2m^*}[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}]\psi(x,y)+V(x,y)\psi(x,y)=E\psi(x,y) \qquad (3)$$

Now, one considers a superposition of a finite number N of plane wave in two-dimensions,

$$\psi(x,y)=\sum_{s=1}^{N}c_s\exp(i\alpha_s x+i\beta_s y) \qquad (4)$$

Where $$\alpha_s{}^2+\beta_s{}^2=\lambda=\frac{2m^*E_s}{\hbar^2} \qquad (5) \qquad s=1,2.......N$$

One applies a mathematical lemma to obtain the coefficients α_s,β_s and the energy levels λ. One considers a set of particular tilings of the plane which are obtained by reflections of a single fundamental region. Using this procedure, one can generate a parallelogram of the plane starting from the reference tilt and reflecting it successfully in its side.

Let a_i and a_j are two adiacent sides of lengths L (a_i) and L(a_j) respectively. Let ζ and η are the reference to coordinate axes which must satisfy the translation[33]

$$\zeta^{'}=\zeta+p_iL(a_i), \qquad \eta^{'}=\eta \qquad (6)$$

And

$$\zeta^{'}=\zeta, \qquad \eta^{'}=\eta+p_jL(a_j) \qquad (7)$$

where p_i and p_j are integers. Considering the smallest p_i and p_j in equation (6) and (7), minimal parallelogram is defined corresponding to each pair of adjacent sides. Workers[38,39] have used this procedure to generate convex plane polygons. In terms of Cartesian coordinate axes x and y, if δ is the angle between a_i and a_j, the two independent translations can be written as

$$x' = x + P_i L(a_i), \qquad y' = y \qquad (8)$$

and $$x' = x + p_i L(a_i)\cos\delta, \quad y' = y + p_j L(a_j)\sin\delta \qquad (9)$$

With respect to equations (4) to (9), the wave functions and energy levels can be written as

$$\psi(x,y) = \exp(\alpha x + \beta y) \qquad (10)$$

Where

$$\alpha = \frac{2n\pi}{p_i L(a_i)} \qquad (11a)$$

$$\beta = \frac{2m\pi\, p_i L(a_i) - 2n\pi\, p_j L(a_j)\cos\delta}{p_i p_j L(a_i) L(a_j)\sin\delta} \qquad (11b)$$

The corresponding eigenvalues are given by

$$\frac{2m^* E(n,m)}{\hbar^2} = \alpha^2(n,m) + \beta^2(n,m) \qquad (12)$$

Using geometrical consideration, the eigenvalues and eigenfunctions for quantum wire with a parallelogram cross-section can be written as

$$\psi_{n,m}(x,y) = \sin[\frac{2\pi\sqrt{3}}{3L} nx]\sin[\frac{2\pi}{3L} my] - (-1)^{(m+2)/2}\sin[\frac{2\pi\sqrt{3}}{3L}\frac{(m+n)}{2}x]$$
$$\sin[\frac{2\pi}{3L}\frac{(3n-m)}{2}y] + (-1)^{(m+n)/2}\sin[\frac{2\pi\sqrt{3}}{3L}\frac{(n-m)}{2}x]\sin[\frac{2\pi}{3L}\frac{(3n+m)}{2}x] \qquad (13)$$

and

$$E(n,m) = (\frac{2\pi^2\hbar^2}{9L^2 m^*})(3n^2 + m^2) \qquad (14)$$

where L is the side length. In the above equation, m and n are integers and have the following conditions

$$n \neq 0, \quad m \neq 0, \quad m \neq \pm 3n, \quad m \neq \pm n \qquad (15)$$

An evaluation of refractive index changes:

In order to calculate refractive index changes of a quantum wire with parallelogram cross section. One uses density matrix formulation. This is related to an optical inter subband transition. As one knows that the system under study can be excited by an electromagnetic field of frequency ω such that

$$E^{\rightarrow}(t) = E^{\rightarrow} e^{i\omega t} + E^{\rightarrow *} e^{-i\omega t} \qquad (16)$$

The time evaluation of the matrix elements of the one-electron density operator ρ can be written as[27,28]

$$\frac{\partial \rho}{\partial t} = \frac{1}{i\hbar}[H_0 - qxE(t), \rho] - \Gamma(\rho - \rho^{(0)}) \qquad (17)$$

Where H_0 is the Hamiltonian of the system without electromagnetic field E (t) and q is the electronic charge. The symbol [,] is the quantum mechanical commutator, $\rho^{(0)}$ is the unperturbed density matrix operator, Γ is the phenomenological operator responsible due to the electron-phonon interaction, collisons among electrons, and etc. It is assumed that Γ is a diagonalized matrix and its elements are equal to the inverse of relaxation time T. In order to solve equation (17), one[38] uses the standard iterative method by expanding ρ

$$\rho(t) = \sum_n \rho^{(n)}(t) \qquad (18)$$

Inserting equation (18) into (17), one can obtain density matrix elements as given below

$$\frac{\partial \rho^{(n+1)}{}_{ij}}{\partial t} = \frac{1}{i\hbar}[H_0, \rho^{(n+1)}]_{ij} - \Gamma_{ij}\rho^{(n+1)}{}_{ij} - \frac{1}{i\hbar}[qx, \rho^{(n)}]_{ij} E(t) \qquad (19)$$

After obtaining the density matrix ρ, one calculates[39] the electronic Polarization P(t) and susptibility $\chi(t)$

$$P(t) = \varepsilon_0 \chi(\omega) E^{\rightarrow} e^{-i\omega t} + \varepsilon_0 \chi(-\omega) E^{\rightarrow *} e^{i\omega t}$$

$$= \frac{1}{V} Tr(\rho M) \qquad (20)$$

Where ρ and V are one-electron density matrix and the volume of the system, ε_0 is the permittivity of free space, and the symbol; Tr (trace) denotes the summation over the diagonal elements of the matrix, M is the dipole moment. One can obtain analytical forms[40] of the linear $\chi^{(1)}$ and the third –order nonlinear $\chi^{(3)}$ susceptibility coefficients using equation (20) and (21). One determines the refractive index changes using the real part of the susceptibility as

$$\frac{\Delta n(\omega)}{n_r} = \mathrm{Re}[\frac{\chi(\omega)}{2n^2{}_r}] \qquad (21)$$

where n_r is the refractive index. The linear and the third-order nonlinear refractive index changes can be expressed as[40]

$$\frac{\Delta n^{(1)}(\omega)}{n_r} = \frac{\sigma_v |M_{21}|^2}{2n^2{}_r\varepsilon_0}[\frac{(E_{21}-\hbar\omega)}{(E_{21}-\hbar\omega)^2+(\hbar\Gamma_{21})^2}] \qquad (22)$$

And

$$\frac{\Delta n^{(3)}(\omega)}{n_r} = -\frac{\sigma_v |M_{21}|^2}{4n^2{}_r\varepsilon_0}[\{\frac{\mu c I}{((E_{21}-\hbar\omega)^2+(\hbar\Gamma_{21})^2)^2}\} \quad x\{4(E_{21}-\hbar\omega)|M_{21}|^2 - \frac{(M_{21}-M_{11})^2}{(E_{21})^2+(\hbar\Gamma_{12})^2}$$
$$x['(E_{21}-\hbar\omega)[''E_{21}(E_{21}-\hbar\omega)-(\hbar\Gamma_{12})^2]'' \; -(\hbar\Gamma_{12})^2(2E_{21}-\hbar\omega)]'\}] \qquad (23)$$

Where σ_v is the carrier density, μ is the permeability, $E_{ij} = E_i - E_j$ is the energy difference, $M_{ij} = |\langle\psi_i|qx|\psi_j\rangle|$ is the matrix element of electric dipole moment. In this work, one has selected the polarization of the electric field in the x-direction. Using equations (21), (22) and (23), one can write the total refractive index changes as

$$\frac{\Delta n(\omega)}{n_r} = \frac{\Delta n^{(1)}(\omega)}{n_r} + \frac{\Delta n^{(3)}(\omega)}{n_r} \qquad (24)$$

RESULTS AND DISCUSSION:

Using the theoretical formalism of Reza Khordad[33] and R. Khordad etal[34], we have theoretically studied inter subband optical properties of quantum wire. We have performed three problems related to the total refractive index changes as a function of photon energy (i) by keeping length and incident optical intensity fixed (ii) by keeping length of the wire fixed and varying incident optical intensities (iii) by keeping incident optical intensity fixed and varying the length of the wire. The evaluated results are shown in **table T1, T2 and T3** respectively. The numerical calculations were carried out by taking the parameters for GaAs parallelogram quantum wire. $n_r = 3.2$, $T_{12} = 0.2$ps, $\Gamma_{12} = 1/T_{12}$, $\sigma_v = 3.0\text{x}\ 10^{16}$ cm^{-3}. Here n_r is the refractive index, σ_v is the carrier density, Γ is diagonal zed matrix and T is the relaxation time. **In table T1,** we have presented the linear, nonlinear and total refractive index changes as a function of photon energy with incident optical intensity I = 0.4 MW/cm^2 and L=10nm. The linear and nonlinear contributions are found opposite in nature. Therefore the total refractive index changes decreases with increase of photon energy. From this calculation, it also appears that the nonlinear term is strongly dependent on the incident optical intensity. **In table T2,** we have shown the evaluated results of total refractive index changes as a function of photon energy by keeping length of the wire fixed and varying the incident optical intensities. We have kept L=10nm fixed and Varied I =0, 0.1, 0.2 and 0.3 MW/cm^2. Our evaluated results show that total refractive index changes decreases with increase of optical intensity. This is quite apparent because the linear term is independent of optical intensity while nonlinear depends strongly. **In table T3,** we have evaluated the total refractive index changes keeping optical intensity fixed and varying the length of the wire. We have kept optical intensity I=0.4 MW/cm^2 and taking L=10, 11, 12 and 15nm. Our theoretically evaluated results indicate that the total refractive index changes decreases as the quantum size L decreases. This is because the refractive index is dependent on the dipole matrix element M_{ij}. By decreasing L_i the wave functions associated with the electron is more compressed and localized. Therefore the dipole moment and thereby, the total refractive index changes reduce. The main reason for this behaviour is the increase of the quantum confinement with decreasing L. Also the energy difference between two electronic states increase by decreasing the length L. There is some recent calculations[41,42] which also reveals the identical behaviour.

CONCLUSION:

From the above investigations and theoretical analysis, we have come across the following conclusions:

(1)We have theoretically evaluated the linear, nonlinear and total refractive index changes as a function of photon energy. We observed that linear and nonlinear contribution of refractive index changes are opposite in nature.

(2)Our theoretical results indicate that total refractive index changes with length of the wire and also with change of incident optical intensities.

(3)We observed that the total refractive index changes reduce when the incident optical intensity increases.

(4)We also observed that the total refractive index changes decrease with decrease of the quantum size of the wire L. This is because the energy difference between two electronic states increases by decreasing L.

(5)These calculations confirm that both the incident optical intensity and structure parameter L has great effects in the refractive index of the wire. These findings can be utilized in quantum confinement of the charge carriers in nano structured material.

Table T1: An evaluated result of linear, nonlinear and total refractive index changes as a function of photon energy (meV) with incident optical intensity I=0.4MW/cm^2 and L=10nm

Photon energy	<-----Refractive index changes------------→		
meV	Linear	nonlinear	Total
5	0.0125	0.0035	0.0160
10	0.0147	0.0058	0.0205
15	0.0228	0.0002	0.0230
20	0.0286	-0.0105	0.0181
25	0.0327	-0.0246	0.0081
30	0.0432	-0.0143	0.0289
35	0.0106	0.0055	0.0161
40	0.0052	0.0118	0.0170
45	-0.0467	0.0206	-0.0261
50	-0.0346	0.0156	-0.0190
55	-0.0267	0.0122	-0.0145
60	-0.0186	0.0095	-0.0091
65	-0.0125	0.0072	-0.0053
70	-0.0052	0.0055	0.0003
80	-0.0008	0.0022	0.0014
100	0.0022	0.0004	0.0026

Table T2: An evaluated result of total refractive index changes as a function of photon energy (meV) for different values of incident optical intensities and fixed value of quantum wire length L=10nm.

Photon energy	<-----Total refractive index changes-----------→			
meV	I=0.0MW/cm^2	I=0.1MW/cm^2	I=0.2MW/cm^2	I=0.3MW/cm^2
5	0.0167	0.0145	0.0138	0.0129
10	0.0236	0.0223	0.0207	0.0185
15	0.0328	0.0308	0.0296	0.0288
20	0.0396	0.0389	0.0365	0.0355
25	0.0456	0.0438	0.0414	0.0405
30	0.0230	0.0245	0.0205	0.0189
35	-0.0542	-0.0506	-0.0412	-0.0365
40	-0.0438	-0.0412	-0.0408	-0.0347
45	-0.0305	-0.0326	-0.0302	-0.0288
50	-0.0255	-0.0227	-0.0212	-0.0206
55	-0.0138	-0.0124	-0.0118	-0.0105
60	-0.0086	-0.0078	-0.0067	-0.0058
65	-0.0052	-0.0046	-0.0039	-0.0032
70	-0.0009	-0.0005	-0.0004	-0.0002
80	0.0014	0.0028	0.0032	0.0044
100	0.0026	0.0047	0.0056	0.0068

Table T3: An evaluated result of total refractive index changes as a function of photon energy (meV) for different values of quantum wire length L with fixed value of incident optical intensity I=0.4MW/cm^2

Photon energy (meV)	<----Total refractive index changes---------→			
	L =10nm	L =11nm	L =12nm	L =15nm
5	0.0244	0.0288	0.0348	0.0689
10	0.0287	0.0358	0.0395	0.0738
15	0.0326	0.0434	0.0486	0.0759
20	0.0445	0.0503	0.0558	0.0695
25	0.0489	0.0544	0.0648	0.0687
30	0.0566	0.0638	-0.0554	-0.0632
35	0.0627	0.0605	-0.0508	-0.0614
40	0.0542	-0.0587	-0.0486	-0.0608
45	-0.0633	-0.0554	-0.0442	-0.0586
50	-0.0615	-0.0517	-0.0402	-0.0554
55	-0.0602	-0.0488	-0.0382	-0.0509
60	-0.0584	-0.0422	-0.0367	-0.0482
65	-0.0502	-0.0408	-0.0342	-0.0453
70	-0.0438	-0.0392	-0.0308	-0.0428
80	-0.0337	-0.0316	-0.0287	-0.0408
90	-0.0274	-0.0258	-0.0264	-0.0395
100	-0.0255	-0.0212	-0.0227	-0.0355

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