OPTICAL ABSORPTION IN AN INDIRECT-GAP SEMICONDUCTOR QUANTUM WELL SYSTEMS

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ABSTRACT

We have derived the optical absorption coefficient due to phonon-assisted, excitonic transitions of a semiconductor layered quantum well (QW) and quantum well wire (QWW) systems having an indirect-band-gap. The spectral dependence of the absorption coefficient varies as \((\hbar \omega \pm M^2 - E_G + E_x)^2\), where \(h\omega(M)\) is the photon (phonon) energy, \(E_G\) is the effective indirect band gap and \(E_x^2\) is the exciton binding energy. \(\beta\) takes the values \(-\frac{1}{2}\), 0 and \(\frac{1}{2}\) for 1D (one-dimensional), 2D and 3D structure systems. Our results for 1D and 2D converge to each other in the appropriate limits and also to 3D (bulk) limit as well. The analytical forms of the exciton-photon and exciton-phonon matrix elements involved in the excitonic transitions in each case are given. The dominant transition mechanism leads to a final indirect bound exciton state assisted by optical phonons in both QW's. Numerical Application taking the parameters of SiGe heterostructures shows that, near the threshold the indirect exciton absorption coefficient in QW, \(\alpha^{[II]}\) is one and two orders of magnitude larger than that of QW, \(\alpha^{[II]}\) and of bulk, \(\alpha^{[III]}\), respectively. On the other hand, \(\alpha^{[V]}\) is bigger than \(\alpha^{[II]}\) by one order of magnitude. These enhancement of \(\alpha^{[II]}\) and \(\alpha^{[V]}\) is function of the dimension of the system and reflects the additional lateral confinement of the carriers in the QW's.

MIRAMARE - TRIESTE
August 1993

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where we have neglected the small second term due to its large energy denominator.

The main notations in Eq.(1) are defined as follows:

$\langle e_x|y - Q(q)|e_x'\rangle$ is the exciton-phonon matrix element

$\langle e_x|y - g |e_x'\rangle$ is the exciton-photon matrix element

$\eta$ and $\xi$ are the phonon and photon polarizations

$E_{ex}$ ($E_{ex}'$) is the energy of the final (intermediate) exciton state

$\mathbf{k}_x (\mathbf{q})$ is the exciton (phonon) wave vector, ($\mathbf{k}_x = \pm \mathbf{q}$).

The other parameters have their standard notations.

The model we adopted in the calculation is a 3-band model (Fig.1) consists of a parabolic valence, intermediate and conduction bands in the vicinity of the band extrema.

The maximum of the valence - and the minimum of the conduction-band occur at $k = 0$ while the minimum of the conduction-band occur at $k = k_{ex}$.

A. 1D (QWW)

We have taken the axis of the wire to be the $z$-direction in our coordinate system and a rectangular cross-section of sides $L_x$ and $L_y$. Therefore, the carriers are confined in two spatial directions $(x, y)$, while they are moving free in the third one ($z$). We assume, potential barriers of infinite height in the $z$-direction and the potential profile of a rectangular QW in the $y$-direction.

For allowed transitions, one can use the effective mass approximation [12] to obtain the wave functions and energy eigenvalues of an exciton state confined in a QWW as

$$\Psi_{ex} = \frac{1}{L_x L_y} U(r_z) \phi_{ex}(r_x, r_y) \phi_{ex}(r_x, r_y) \phi_{ex}(r_x, r_y) \phi_{ex}(r_x, r_y)$$

which is the superposition of Bloch states for the electron (with position vector $r_x$) in the conduction band and the hole (with position vector $r_y$) in the valence band.

$U(r_z)$ is the relative motion wavefunction of the electron and hole along the wire.

$\phi_{ex}(r_x, r_y)$ are the $xy$-wavefunctions of the quantum numbers $n/2$ and $n'/(n/2)$ electron (hole) subbands

$$E_{ex}(\mathbf{r}) = E_g + \frac{\hbar^2 k_x^2}{2m_{ex}(\mathbf{r})} + E_{ex}^{(1)}$$

where $E_g$ is the indirect energy gap and $\mu_{ex}(\mathbf{r})$ is the exciton reduced mass for the motion along $xy$-plane formed from the hole in the valence band and the electron in the conduction (intermediate) band.

$$E_{ex}^{(1)} = \epsilon_{ex}^{(1)}(n_x^2 + n_y^2) + \epsilon_{ex}^{(1)}(\ell^2 + \ell'^2)$$

with

$$\epsilon_{ex}^{(1)}(n_x^2 + n_y^2) = \frac{\pi^2 \hbar^2}{2m_{ex}(\mathbf{r}) L_x^2}$$

and

$$\epsilon_{ex}^{(1)}(\ell^2 + \ell'^2) = \frac{\pi^2 \hbar^2}{2\mu_{ex}(\mathbf{r}) L_y^2}$$

are the quantized exciton energies.

Substituting from Eqs.(2) and (3) into (1) and performing the integration, one obtains the following expression for the indirect exciton absorption coefficient assisted by optical phonons in QWW's.

$$\alpha_{\omega}^{(1)}(x) = \frac{C_1}{\omega} \sum_{\alpha \neq \alpha'} |N_1 M_1 \Gamma_1|^2 \left( n(\Omega_{\alpha}) + \frac{1}{2} \right)$$

$$\times \left\{ (\hbar \omega + \hbar \Omega - E_G + E_{ex}') + \Theta(\hbar \omega + \hbar \Omega - E_G + E_{ex}) \right\}$$

$$\delta(\hbar \omega + \hbar \Omega - E_G + E_{ex}')$$

$\Theta(\hbar \omega + \hbar \Omega - E_G + E_{ex})$ (4)

where

$$C_1 = \frac{\epsilon_{ex}^{(1)}(\ell^2 + \ell'^2)}{2\pi^2 \hbar c n^2}$$

$\mu_{ex}^{(2)}$ is the exciton reduced mass for the motion along $xy$ plane and $s$ is the refractive index at frequency $\omega$.

$N_1$ is the temperature independent part of the exciton-phonon matrix element (see the Appendix).

$$M_1 = \sum_{\alpha, \beta, \beta'} (\mathbf{u}_n(\mathbf{r}, \ell, \beta) \cdot \mathbf{p}_n \mathbf{u}_{n'}(\mathbf{r}, \ell', \beta')) \delta(\mathbf{p}_n + \mathbf{p}_{n'})$$

where $\mathbf{u}_n(\mathbf{r}, \ell, \beta)$ is the Bloch function of the valence band in the $xy$-plane and the summation is over the electron in the conduction band and the heavy hole $(hh)$ and light hole $(lh)$ of the valence band. $U(0)$ is the exciton envelope function for zero relative motion.

$\eta(\Omega_{\alpha}) = 1 / \exp(\hbar \Omega_{\alpha} / k_B T_1) - 1$ is the Bose-Einstein distribution function for phonon of wave vector $q$. The upper (lower) sign indicates that phonon is absorbed (emitted)

$$E_G = E_g + E_{ex}' + \Theta(\hbar \omega + \hbar \Omega - E_G)$$

$s = 1/(\hbar \omega - E_G' - E_{ex}')$ where $E_G'$ is the direct gap.

B. 2D (QW)

For the same band model (Fig.1) and assuming that the carriers are quantized along the $z$-direction and are free to move in the $xy$-plane. For infinite potential barriers the exciton wavefunctions and energy levels are given by

$$\Psi_{ex} = \frac{1}{L_x L_y} U(r_z) \phi_{ex}(r_x, r_y) \phi_{ex}(r_x, r_y) \phi_{ex}(r_x, r_y)$$

$L_z$ is the width of the QW. $U(r_z)$ is the two dimensional exciton envelope function which represents the relative motion along the $xy$-plane. $\phi_{ex}(\mathbf{r})$ is the envelope function of the electron (hole) of the quantum number $n/2$ (n/2) subbands.

$$\Psi_{ex} = \frac{1}{L_x L_y} U(r_z) \phi_{ex}(r_x, r_y) \phi_{ex}(r_x, r_y)$$

$$\phi_{ex}(r_x, r_y) = \frac{1}{L_x L_y} U(r_z) \phi_{ex}(r_x, r_y) \phi_{ex}(r_x, r_y)$$

$$\phi_{ex}(r_x, r_y) = \frac{1}{\hbar^2 (n_x^2 + n_y^2) + \epsilon_{ex}^{(2)}}$$

$$E_{ex}(\mathbf{r}) = E_g + \frac{\hbar^2 k_x^2}{2m_{ex}(\mathbf{r})} + E_{ex}^{(2)}$$

where

$$\epsilon_{ex}^{(2)} = \epsilon_{ex}^{(2)}(n_x^2 + n_y^2) + \epsilon_{ex}^{(2)}(\ell^2 + \ell'^2)$$

are the quantized exciton energies.
By inserting Eqs.(5) and (6) into (1) we obtain for the phonon-assisted absorption coefficient in layered QWs

\[
\alpha_{\text{ex}}^{(2)}(\omega) = \frac{C_2}{\omega} \sum_{\omega, n} \left| N_2 M_2 \Gamma^2 (n) \left( \frac{\Omega e + \frac{1}{2} + \frac{1}{2}n^2}{2} \right) \right| \times \begin{cases} \Theta(\hbar \omega - n \Omega - E_G + E_{\gamma}^{(2)}) \quad (\hbar \omega - n \Omega \geq E_G) \\ \delta(\hbar \omega - n \Omega - E_G + E_{\gamma}^{(2)}) \quad (\hbar \omega - n \Omega < E_G) \end{cases} \]

where \( C_2 = e^2 \mu^* \gamma s / 4 \pi^2 \hbar^2 \) and \( \mu^* \) is the exciton reduced mass of the motion along z-axis. \( N_2 \) is the matrix element of the exciton-phonon operator in QW (see the Appendix). 

\[
M_2 = \sum_{\epsilon, n, \ell, \ell'} \langle \epsilon|u(\tilde{r}_s - \tilde{r}_a)|n, \ell, u(\tilde{r}_a) \rangle \langle n|u_s(\tilde{r}_a)|\psi_{\gamma}(\tilde{r}) \rangle \langle \psi_{\gamma}|u_s(0)|u_s(0) \rangle
\]

\[
\Gamma_2 = \frac{1}{(\hbar \omega - E_G - E_{\gamma}^{(2)})}, \quad E_G = E_G + E_{\gamma}^{(2)}
\]

\( u_s \) is a Bloch function of the valence band along z-axis. \( \gamma \) is a 2D wave vector in the xy-plane.

C. 2D (bulk)

The exciton wavefunctions and energy eigenvalues, in this case, are

\[
\Psi_{\text{ex}} = U(|\epsilon| - r_s)\psi_{\gamma}(\tilde{r}) u_s(\tilde{r}_a)
\]

\[
E_{\text{ex}(\epsilon)} = E_G + \frac{\hbar^2 \gamma^2}{2 \mu^*} \epsilon^2
\]

The absorption coefficient for indirect exciton in bulk semiconductors becomes

\[
\alpha_{\text{ex}}^{(2)}(\omega) = \frac{C_3}{\omega} \sum_{\epsilon, n, \ell, \ell'} \langle \epsilon|u(\tilde{r}_s - \tilde{r}_a)|n, \ell, u(\tilde{r}_a) \rangle \langle n|u_s(\tilde{r}_a)|\psi_{\gamma}(\tilde{r}) \rangle \langle \psi_{\gamma}|u_s(0)|u_s(0) \rangle \times \begin{cases} \Theta(\hbar \omega - n \Omega - E_G + E_{\gamma}^{(2)}) \quad (\hbar \omega - n \Omega \geq E_G) \\ \delta(\hbar \omega - n \Omega - E_G + E_{\gamma}^{(2)}) \quad (\hbar \omega - n \Omega < E_G) \end{cases}
\]

where

\[
C_3 = e^2 \mu^* \gamma s / 2 \pi^2 \hbar^2 \epsilon^2 \gamma^2
\]

\( N_3 \) is the exciton-phonon matrix element in bulk materials

\[
M_3 = \sum_{\epsilon, n, \ell, \ell'} \langle \epsilon|u(\tilde{r}_s - \tilde{r}_a)|n, \ell, u(\tilde{r}_a) \rangle \langle n|u_s(\tilde{r}_a)|\psi_{\gamma}(\tilde{r}) \rangle \langle \psi_{\gamma}|u_s(0)|u_s(0) \rangle
\]

\[
\Gamma_3 = 1/(\hbar \omega - E_G)
\]

3 Results and Discussion

At photon energies before the threshold the indirect absorption coefficients \( \alpha_{\text{ex}}^{(1)} \), \( \alpha_{\text{ex}}^{(2)} \) and \( \alpha_{\text{ex}}^{(3)} \) lead to a final exciton state via an s type exciton as intermediate state.

After the band edge, we note that \( \alpha_{\text{ex}}^{(1)} \), \( \alpha_{\text{ex}}^{(2)} \) and \( \alpha_{\text{ex}}^{(3)} \) are directly proportional to the density of the electron-hole pairs created by the absorption of a photon or emission of absorption of a photon. These expressions are found to vary according to \( (\hbar \omega - \Omega - E_G + E_{\gamma}^{(2)})^{\beta} \) where the exponent \( \beta \) takes the values \(-\frac{1}{2}, 0, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \frac{9}{2} \) for 1D, 2D, 3D and bulk systems respectively. \( \alpha_{\text{ex}}^{(2)} \) can be obtained by replacing the summation over \( \ell \) and \( \ell' \) in Eq.(4), by integration over these quantum numbers. In the same way, \( \alpha_{\text{ex}}^{(3)} \) can be obtained by replacing the summation over \( n \) and \( n' \) in Eq.(7) by integrations.

Eq.(4) for 1D case shows, at the threshold, a series of peaks occur whenever phonon can assist transition between a given pair of subbands in the initial and final bands having the same subband quantum numbers \( n \) and \( \ell \). The position of these peaks shift to higher energies as the lateral dimension of the wire decreases (as shown in Fig.2).

In the case of 2D system, \( \alpha_{\text{ex}}^{(2)} \) as function of \( \hbar \omega \) consists of a series of steps with a new step coming in whenever there is a transition between the quantized subbands in the conduction and valence bands with the emission or absorption of a phonon. The lower energy step occurs when a phonon is being absorbed, while the higher-energy step occurs for phonon emission. The position of these steps will shift to higher energies as the width of the QW decreases (Fig.3).

In Fig.4 we show, for comparison, \( \alpha_{\text{ex}}^{(2)} \) for bulk materials which behaves [13] as the square root of the threshold energy as function of \( \hbar \omega \).

The band edge for exciton absorption to occur is shifted to higher photon energies as going from bulk to 2D to 1D structures. This is due to the increase of the effective indirect band gap with the size quantization of the excitonic energy levels.

All the three \( \alpha_{\text{ex}}^{(n)} \) are function of the temperature \( T \) through the Bose-Einstein term, \( \frac{\rho(T)}{\epsilon^2} \). At high temperatures transition can occur with the emission and absorption of phonons while at low temperatures, where there are few phonons available of wavevector needed for the phonon-assisted transitions, transitions can only occur with the emission of a phonon.

The polarization dependence of the absorption coefficients is maintained in the inter-subband exciton-phonon matrix elements.

Numerical calculation taking the parameters [14] of Si0.2Ge0.8 shows that \( \alpha_{\text{ex}}^{(1)} \) at the vicinity of the band edge is two (one) orders of magnitude larger than \( \alpha_{\text{ex}}^{(2)}(\alpha_{\text{ex}}^{(3)}) \). Furthermore, \( \alpha_{\text{ex}}^{(2)} \) is only one order of magnitude larger than \( \alpha_{\text{ex}}^{(3)} \). This enhancement is due to the carriers confinement in the QW and the additional lateral confinement inside the QW and bulk structures.

4 Conclusion

Phonon-assisted excitonic transitions in QWW, layered QW and bulk semiconductor structures have been theoretically investigated. The spectral dependence of the absorption coefficients for the exciton, after the edge, are directly proportional to \( (\hbar \omega - \Omega - E_G + E_{\gamma}^{(2)})^{\beta} \), where \( \beta \) takes the values \(-\frac{1}{2}, 0, \frac{1}{2}, \frac{3}{2} \) for 1D, 2D and 3D cases respectively. These expressions are found to converge to each other under the appropriate limits. The
transitions lead to a final exciton state of s-type symmetry via an intermediate exciton of the same symmetry. Numerical calculation for the case of SiGe shows that $\alpha^{(1)}$ is enhanced over $\alpha^{(2)}$ and $\alpha^{(3)}$ by one and two orders of magnitude respectively. This result reflects the additional lateral confinement of the carriers inside the QWW. On the other hand, $\alpha^{(2)} > \alpha^{(3)}$ by only one order of magnitude which is the result of less confinement in QW's.

**Acknowledgments**

The author would like to thank Professor Abdus Salam, the International Atomic Energy Agency and UNESCO for hospitality at the International Centre for Theoretical Physics, Trieste.

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**Appendix**

**Exciton-phonon matrix element**

In bulk materials (3D), the electron-phonon interaction operators can be written in the form [13]

$$Q(\vec{r}) = \sum_{\vec{q}} D_\vec{q} \exp(i\vec{q} \cdot \vec{r}) [a(\vec{q}) + a^+(\vec{q})]$$

where $D_\vec{q}$ is the lattice deformation potential, $\vec{q}$ is the 3D phonon wave vector and $a, a^+$ are the phonon annihilation and creation operators.

The hole-phonon interaction differs from the above expression only by a change of sign corresponding to the positive charge of the hole. Transforming to center-of-mass coordinates for the exciton, the exciton-phonon interaction reads

$$Q(\vec{r}) = \sum_{\vec{q}} D_\vec{q} \exp(i\vec{q} \cdot \vec{R}) \{\exp(iM_\vec{q} \cdot \vec{r} - \exp(-iM_\vec{q} \cdot \vec{r})\} \times$$

$$\times [a(\vec{q}) + a^+(\vec{q})]$$

where

$$\vec{R} = \frac{m_s \vec{r}_s + m_h \vec{r}_h}{m_s + m_h}, \quad \vec{r} = \vec{r}_s - \vec{r}_h$$

and $M_{\vec{q}} = m_s / (m_s + m_h)$

**1D case**

For optical phonons the exciton-phonon matrix element becomes, (for excitons with envelope function at zero relative motion)

$$| \vec{N}_1 |^2 = |\langle \Psi_2(\vec{r}, x, y) | \vec{q} \cdot \vec{Q} | \Psi_s(\vec{r}, x, y) \rangle |^2$$

$$= \frac{1}{2\rho V_0} \int J(q_x, \Omega_0) U_{s,h}(0) U_{s,h}^*(0) \Omega_0 \Omega_0 | \Omega_0 |^2$$

where

$$J(q_x, \Omega_0) = \int_0^{k_s} \int_0^{k_h} \sin k_x x \sin k_y y \sin k_z z \exp(ik_x x + ik_y y + ik_z z) \, dx \, dy$$

$U_{s,h}$ and $U_{s,h}^*$ are the final and intermediate exciton envelope functions respectively ($\vec{R}_{s,h} = \vec{K}_s - \vec{K}_h$)

**2D Case**

In this case we have

$$| \vec{N}_2 |^2 = |\langle \Psi_2(\vec{r}, z) | \vec{q} \cdot \vec{Q} | \Psi_s(\vec{r}, z) \rangle |^2$$
\[ \frac{h D_2}{2 \rho \Omega V_0} \left| J(q) U_{x,a}(0) U_{y,a}^*(0) \right|^2 \left( \frac{\Omega}{2} + \frac{1}{2} \right) \]

where \( V_0 \) is the volume of the QW,

\[ J(q) = \int_0^{L_z} \sin k_z' z \sin \theta q_z' e^{i \theta q_z' z} \, dz \]

and \( q \) is a 2D wave vector.

3D Case

For bulk semiconductors, one obtains for the exciton-phonon matrix elements

\[ |\tilde{N}_3|^2 = |\langle \Psi_{\tilde{p}}(\tilde{q}) | \vec{\tilde{q}} \cdot \hat{\vec{q}} | \Psi_{\tilde{p}}(\tilde{q}) \rangle|^2 \]

\[ = \frac{h D_2}{\rho \Omega V_0} \left| J(q) U_{x,a}(0) U_{y,a}^*(0) \right|^2 \left( \frac{\Omega}{2} + \frac{1}{2} \right) \]

where

\[ J(q) = \int e^{i \theta q} \, d\vec{r} \]

and \( q \) is a 3D wave vector.

References


L. A. Coldren and P. M. Petroff, Phys. Rev. Lett. 62, 466 (1989);


[7] see e.g. B.K. Ridley, Quantum Processes in Semiconductors (Clarendon Oxford 1982).

[8] Luryi and S.M. Sze, in Silicon Molecular Beam Epitaxy CRC Uniscience Series edited by E. Kasper and J.C. Beam (1988);


S.C. Jain and W. Hayes, Semicond. Sci. Technol. 6, 347 (1991);

Figure Captions

Fig. 1 Schematic diagram of the 3-band model used in the calculation for α_{rr}'s in an indirect-band-gap semiconductor QWW, QW and bulk structures. The arrows indicate the coupling matrix elements included in each step process. Dashed lines are the quantized energy levels while the solid lines are the exciton states.

Fig. 2 α_{zz}^{(1)} for QWW as function of the photon energy ħω at L_x = L_y = 200 Å (solid curve) and at L_x = L_y = 100 Å (dashed curve). We used the parameters characteristic of Si_{0.5}Ge_{0.5}: m_{1}^* = 0.19m_0, m_{2}^* = 0.49m_0, E_g = 1.02 eV, hΩ = 60 meV, E_{v} = 10 meV [Ref.14].

Fig. 3 α_{zz}^{(2)} for layered QW as function of the photon energy ħω at L_z = 200 Å (solid line) and L_z = 100 Å (dashed line) for the same compound.

Fig. 4 α_{zz}^{(3)} for bulk case as function of the photon energy.
Fig. 2

First subband

Second subband

Phonon Absorption

Phonon Emission

\( \omega = \hbar \omega_{\text{ph}} - E_{\text{ex}}^{b} \)

\( \omega = \hbar \omega_{\text{ph}} + E_{\text{ex}}^{b} \)

Fig. 3

First Subband

Phonon Absorption

Second Subband

Phonon Emission

\( \omega = \hbar \omega_{\text{ph}} - E_{\text{ex}}^{b} \)

\( \omega = \hbar \omega_{\text{ph}} + E_{\text{ex}}^{b} \)