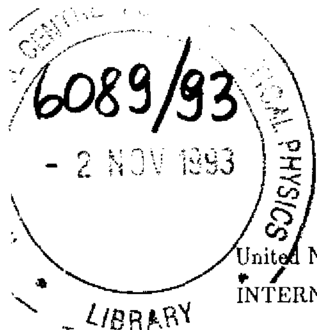

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OPTICAL ABSORPTION IN AN INDIRECT-GAP SEMICONDUCTOR QUANTUM WELL SYSTEMS

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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 coefficients varies as $(\hbar\omega \pm \hbar\Omega - E_G + E^b_{ex})^\beta$, where $\hbar\omega(\hbar\Omega)$ is the photon (phonon) energy, E_G is the effective indirect band gap and E^b_{ex} is the exciton binding energy, β 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 lead to a final indirect bound 1s exciton state assisted by optical phonons in both QW's. Numerical Application taking the parameters of $Si_{0.5}Ge_{0.5}$ shows that, near the threshold the indirect exciton absorption coefficient in QWW, $\alpha^{(1)}_{ex}$ is one and two orders of magnitude larger than that of QW, $\alpha^{(2)}_{ex}$ and of bulk, $\alpha^{(3)}_{ex}$, respectively. On the other hand, $\alpha^{(2)}_{ex}$ is bigger than $\alpha^{(3)}_{ex}$ by one order of magnitude. These enhancement of $\alpha^{(1)}_{ex}$ and $\alpha^{(2)}_{ex}$ is function of the dimension of the system and reflects the additional lateral confinement of the carriers in the QWW's.

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1 Introduction

The advantages of epitaxial growth techniques allowed the synthesis of artificial quantum well structures with novel optical properties which do not exist in bulk constituents [1]. The optical properties of undoped 2D structures are strongly influenced by the carrier confinement in the growth direction leading to a significant enhancement of the excitonic binding energy [2]. Interest has started to reducing the dimensionality of these structures. There have been several experimental results with [3] and without [4] excitonic effect on laterally patterned structures where an additional laterally confinement appear on top of the QW in the growth direction. In these structures one obtain 1D limit where the valence and conduction subbands have been quantized by lateral confinement. Interband direct optical absorption in semiconductor QWW's has been investigated theoretically for parabolic [5] and non-parabolic and valence mixing bands [6]. Most of the work on QW heterostructures has been performed using GaAs/Ga_{1-x} Al_x As system where GaAs is a direct band-gap semiconductor [7]. A rapid progress in strained layer $Si/Si_{1-x}Ge$ superlattices [8] has substantially enhanced the potential versatility of the Si-based technology. Since silicon is an indirect-band-gap semiconductor, its optical properties are different from GaAs since in the former materials the electronic transitions should be assisted by phonons. The optical absorption due to phonon-assisted interband [9] and excitonic [10] transitions have been calculated for the case where the QW consists of an indirect-gap semiconductors.

The purpose of the present paper is to develop a theory of phonon-assisted excitonic transitions in layered QW and QWW structures made of an indirect-band-gap semiconductors. both the exciton-photon and exciton-phonon matrix elements included in the theory are analytically derived. The optical transitions in bulk materials are also given, for comparison. We have calculated the expressions for the indirect absorption coefficients to exciton states in 1D, 2D and 3D systems. At the vicinity of the band edge our result for 1D and 2D converge to each other in the appropriate limits and also to the result of 3D as well. Numerical estimation shows that the absorption coefficient, near the edge, in QW systems is enhanced over that of bulk materials. This enhancement is found to be due to the strong confinement of the exciton in the QW structures. The spectral dependence of the absorption coefficient is found to obey a law as $(\hbar\omega \pm \hbar\Omega - E_G E^b_{ex})^\beta$ where β is function of the dimension of the system.

The theory is outlined in Sec. II. The results and discussion are given in Sec. III. Sec. IV includes the conclusions.

2 Theory

Phonon-assisted excitonic transitions in an indirect gap semiconductors is a two-step process. Therefore, the transition rate, for an electron to absorb one photon and emitte or absorb a phonon, from the initial ground state $|g\rangle$ to a final exciton state $|ex\rangle$ via an intermediate exciton state $|ex'\rangle$ is given from second-order perturbation theory as [11]

$$W_{ex}(\omega) = \frac{2\pi}{\hbar}(\frac{e}{m_0 c})^2|A_0|^2\frac{V}{(2\pi)^2}\int d\vec{k}_{ex}\left|\frac{\langle ex|\vec{\eta}\cdot\vec{Q}|ex'\rangle ex'|\vec{\varepsilon}\cdot\vec{p}|g\rangle}{(E'_{ex}-\hbar\omega)}\right|^2 \times \times\,\delta(E_{ex}-\hbar\omega\mp\hbar\Omega) \quad (1)$$

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

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

$\langle ex|\vec{\eta}\cdot Q(\vec{q})|ex'\rangle$ is the exciton-phonon matrix element

$\langle ex'|\vec{\varepsilon}\cdot\vec{p}|g\rangle$ is the exciton-photon matrix element

$\vec{\eta}$ and $\vec{\varepsilon}$ are the phonon and photon polarizations

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

$\vec{k}_{ex}(\vec{q})$ is the exciton (phonon) wave vector, ($\vec{k}_{ex} = \pm\vec{q}$).

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 $\vec{k} = 0$ while the minimum of the conduction-band occur at $\vec{k} = \vec{k}_{ex}$.

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 Lx and Ly. 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 x-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

$$\Psi_{ex} = \frac{1}{L_x L_y} U(\vec{r}_z)\phi_{en\ell}(x_e, y_e)\phi_{hn'\ell'}(x_h, y_h)u_c(\vec{r}_e)u_v(\vec{r}_h) \tag{2}$$

which is the superposition of Bloch states for the electron (with position vector $\vec{r}_e$) in the conduction band and the hole (with position vector $\vec{r}_h$) in the valence band.

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

$\phi_{en\ell}$ ($\phi_{hn'\ell'}$) are the xy -wavefunctions of the quantum numbers nth and ℓth ($n'th$ and $\ell' th$) electron (hole) subbands

$$E_{ex(ex')} = Eg + \frac{\hbar^2 k^2_{ex(ex')}}{2\mu_{ex(ex')}} + E^{(1)}_{ex(ex')} \tag{3}$$

where Eg is the indirect energy gap and $\mu_{ex(ex')}$ 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.

$$E^{(1)}_{ex(ex')} = \varepsilon^x_{ex(ex')}(n^2 + n'^2) + \varepsilon^y_{ex(ex')}(\ell^2 + \ell'^2)$$

with

$$\varepsilon^x_{ex(ex')} = \frac{\pi^2\hbar^2}{2\,\mu_{ex(ex')}L_x^2} \text{ and } \varepsilon^y_{ex(ex')} = \frac{\pi^2\hbar^2}{2\mu_{ex(ex')}L_y^2}$$

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.

$$\alpha^{(1)}_{ex}(\omega) = \frac{C_1}{\omega}\sum_{nn'\ell\ell'}|N_1 M_1 \Gamma_1|^2 (n(\Omega_{q_z}) + \frac{1}{2} \mp \frac{1}{2})$$

$$\times \begin{cases} (\hbar\omega \pm \hbar\Omega - E_G + E^b_{ex})^{-\frac{1}{2}}\Theta(\hbar\omega \pm \hbar\Omega - E_G + E^b_{ex}) & (\hbar\omega \pm \hbar\Omega) \geq E_G \\ \delta(\hbar\omega \pm \hbar\Omega - E_G + E^b_{ex}) & (\hbar\omega \pm \hbar\Omega) < E_G \end{cases} \tag{4}$$

where

$$C_1 = \frac{e^2(\mu^{xy}_{ex})^{\frac{1}{2}}}{2^{\frac{5}{2}}\pi^3\hbar c s m_0^2}$$

μ^{xy}_{ex} is the exciton reduced mass for the motion along xy plane and s is the refractive index at frequency ω.

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

$$M_1 = \sum_{e,h(hh,\ell h)} \langle u_c(n,\ell,\vec{k})|\vec{\varepsilon}\cdot\vec{p}|u^{xy}_v(n',\ell',\vec{k})\rangle\langle\phi_{cn}|\frac{\partial}{\partial x}|\phi_{vn'\ell'}\rangle|U_{\ell,h}(\vec{r}=0)|$$

where u^{xy}_v 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.

$n(\Omega_{q_z}) = 1/\exp(\frac{\hbar\Omega_{q_z}}{kT} - 1)$ is the Bose-Einstein distribution function for phonon of wave vector q_z. The upper (lower) sign indicates that phonon is absorbed (emitted) $E_G = Eg + E^{(1)}_{ex}$ $\Theta(x) = \begin{cases} 1 & x>0 \\ 0 & x<0 \end{cases}$ is a unit step function.

$\Gamma_1 = 1/(\hbar\omega - Eg' - E^{(1)}_{ex'})$ where Eg' in 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

$$\Psi_{ex} = \frac{1}{L_z}U(\vec{r}_{xy})\phi_{en}(z_e)\phi_{hn'}(z_n)u_c(\vec{r}_e)u_v(\vec{r}_h) \tag{5}$$

L_z is the width of the QW. $U(\vec{r}_{xy})$ is the two dimensional exciton envelope function which represents the relative motion along the xy-plane. $\phi_{en}(\phi_{hn'})$ is the envelope function of the electron (hole) of the quantum number nth ($n'th$) subbands.

$$E_{ex(ex')} = Eg + \frac{\hbar^2 k^2_{ex}}{2\mu_{ex(ex')}} + E^{(2)}_{ex(ex')} \tag{6}$$

where

$$E^{(2)}_{ex(ex')} = \varepsilon_{ex(ex')}(n^2 + n'^2)$$

with

$$\varepsilon_{ex(ex')} = \frac{\pi^2\hbar^2}{2\mu_{ex(ex')}L_z^2}$$

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

$$\alpha_{ex}^{(2)}(\omega) = \frac{C_2}{\omega}\sum_{n,n'}|N_2M_2\Gamma_2|^2(n(\Omega_{\vec{q}}) + \frac{1}{2} \mp \frac{1}{2})$$

$$\times \begin{cases} \Theta(\hbar\omega \pm \hbar\Omega - E_G + E_{ex}^b) & (\hbar\omega \pm \hbar\Omega) \geq E_G \\ \delta(\hbar\omega \pm \hbar\Omega - E_G + E_{ex}^b) & (\hbar\omega \pm \hbar\Omega) < E_G) \end{cases} \quad (7)$$

where $C_2 = e^2\mu_{ex}^z/4\pi^3 s\hbar^2 cm_0^2$.

μ_{ex}^z 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)

$$M_2 = \sum_{e,h(hh,\ell h)} \langle u_c(n,\vec{k})|\vec{\varepsilon}\cdot\vec{p}|u_v^z(n',\vec{k})\rangle\langle\phi_{en}|\frac{\partial}{\partial z}|\phi_{hn'}\rangle|U_{e,h}(0)|$$

$$\Gamma_2 = 1/(\hbar\omega - E'g - E_{ex'}^{(2)}),\ E_G = Eg\ + E_{ex}^{(2)}$$

u_v^z is the Bloch function of the valence band along z-axis.
$\vec{q}$ is a 2D wave vector in the xy-plane.

C. 2D (bulk)

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

$$\Psi_{ex} = U(\vec{r}_e - \vec{r}_h)u_c(\vec{r}_c)u_v(\vec{r}_h) \quad (8)$$

$$E_{ex(ex')} = Eg + \frac{\hbar^2k_{ex}^2}{2\mu_{ex(ex')}} \quad (9)$$

The absorption coefficient for indirect exciton in bulk semiconductors becomes

$$\alpha_{ex}^{(3)}(\omega) = \frac{C_3}{\omega}|N_3M_3\Gamma_3|^2(n(\Omega_{\vec{q}}) + \frac{1}{2} \mp \frac{1}{2})\times$$

$$\begin{cases} (\hbar\omega \pm \hbar\Omega - E_G + E_{ex}^b)^{\frac{1}{2}}\Theta(\hbar\omega \pm \hbar\Omega - E_G + E_{ex}^b) & (\hbar\omega \pm \hbar\Omega) \geq E_G \\ \delta(\hbar\omega \pm \hbar\Omega - E_G + E_{ex}^b) & (\hbar\omega \pm \hbar\Omega) < E_G \end{cases} \quad (10)$$

where

$$C_3 = \frac{e^2\mu_{ex}^{\frac{3}{2}}}{2^{\frac{3}{2}}\pi^2 sc\hbar^3 m_0^2},\ E_G = Eg$$

N_3 is the exciton-phonon matrix element in bulk materials

$$M_3 = \sum_{e,h(hh,\ell h)} \langle u_c(\vec{k})|\vec{\varepsilon}\cdot\vec{p}|u_v(\vec{k})\rangle$$

$$\Gamma_3 = 1/(\hbar\omega - Eg')$$

3 Results and Discussion

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

After the band edge, we note that $\alpha_{ex}^{(1)}$, $\alpha_{ex}^{(2)}$ and $\alpha_{ex}^{(3)}$ are directly proportional to the density of the electron-hole pairs created by the absorption of a photon and emission or absorption of a phonon. These expressions are found to vary according to $(\hbar\omega \pm \hbar\Omega - E_G + E_{ex}^b)^\beta$ where the exponent β takes the values $-\frac{1}{2}$, 0 and $\frac{1}{2}$ for 1D, 2D and 3D systems respectively. $\alpha_{ex}^{(2)}$ can be obtained by replacing the summation over ℓ and ℓ', in Eq.(4), by integration over these quantum numbers. In the same way, $\alpha_{ex}^{(3)}$ 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 ℓ. 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, $\alpha_{ex}^{(2)}$ 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, $\alpha_{ex}^{(3)}$, 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 α_{ex}'s are function of the temperature T through the Bose-Einstein term, $n(\Omega_{\vec{q}})$. 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-subbant exciton-photon matrix elements.

Numerical calculation taking the parameters [14] of $Si_{0.5}Ge_{0.5}$ shows that $\alpha_{ex}^{(1)}$ at the vicinity of the band edge is two (one) orders of magnitude larger than $\alpha_{ex}^{(3)}(\alpha_{ex}^{(2)})$. Furthermore, $\alpha_{ex}^{(2)}$ is only one order of magnitude larger than $\alpha_{ex}^{(3)}$. This enhancement is due to the carriers confinement in the QW and the additional lateral confinement inside the QWW over the QW and bulk structures.

4 Conclusion

Phonon-assisted excitonic transitions in QWW, layered QW and bulk semiconducture structures have been theoretically investigated. The spectral dependence of the absorption coefficients for the exciton, after the edge, are directly proportional to $(\hbar\omega \pm \hbar\Omega - E_G + E_{ex}^b)^\beta$, where β takes the values $-\frac{1}{2}$, 0 and $\frac{1}{2}$ 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 $Si_{0.5}Ge_{0.5}$ shows that $\alpha_{ex}^{(1)}$ is enhanced over $\alpha_{ex}^{(2)}$ and $\alpha_{ex}^{(3)}$ 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, $\alpha_{ex}^{(2)} > \alpha_{ex}^{(3)}$ by only one order of magnitude which is the result of less confinement in QW's.

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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]

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

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-photon interaction reads

$$Q(\vec{r}) = \sum_{\vec{q}} iD_{\vec{q}} \exp(i\vec{q}\cdot\vec{R})\{\exp(iM_e\vec{q}\cdot\vec{r} - \exp(-iM_h\vec{q}\cdot\vec{r})\}\times$$

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

where

$$\vec{R} = \frac{m_e\vec{r}_e + m_h\vec{r}_h}{m_e + m_h}, \quad \vec{r} = \vec{r}_e - \vec{r}_h$$

and $M_{h,e} = m_{e,h}/(m_e + m_h)$

1D case

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

$$|\vec{N}_1|^2 = |\langle\Psi_{\vec{k}'}(\vec{r},x,y)|\vec{\eta}\cdot\vec{Q}|\Psi_k(\vec{r},x,y)\rangle|^2$$

$$= \frac{\hbar D_0^2}{2\rho\Omega_{q_z}V_0}|J(q_x,q_y)U_{e,h}(0)U'_{e,h}(0)|^2(n(\Omega_{q_z}) + \frac{1}{2} \mp \frac{1}{2})$$

where

D_0 = optical deformation constant for coupling to optical phonon

V_0 volume of QWW, ρ = mass density

$$J(q_x,q_y) = \int_0^{Lx}\int_0^{Ly} \sin k'_x x \sin k' y \sin k_x x \sin k_y y e^{i(q_x x + q_y y)} dx dy$$

$U_{e,n}$ and $U'_{e,h}$ are the final and intermediate exciton envelope functions respectively ($\vec{k}_{ex} = \vec{k}' - \vec{k}$)

2D Case

In this case we have

$$|\vec{N}_2|^2 = |\langle\Psi_{k'}(\vec{r},z)|\vec{\eta}\cdot\vec{Q}|\Psi_k(\vec{r},z)\rangle|^2$$

$$= \frac{\hbar D_0^2}{2\rho\Omega_{\vec{q}}V_0}|J(q_z)U_{e,h}(0)U'_{e,h}(0)|^2(n(\Omega_{\vec{q}}) + \frac{1}{2} \mp \frac{1}{2})$$

where V_0 is the volume of the QW,

$$J(q_z) = \int_0^{L_z} \sin k'_z z \sin k_z z e^{iq_z z} dz$$

and $\vec{q}$ is a 2D wave vector

3D Case

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

$$|\vec{N}_3|^2 = |\langle\Psi_{\vec{k}'}(\vec{r})|\vec{\eta}\cdot\vec{Q}|\Psi_{\vec{k}}(\vec{r})\rangle|^2$$

$$= \frac{\hbar D_0^2}{\rho\Omega\vec{q}V_0}|J(\vec{q})U_{e,h}(0)U'_{e,h}(0)|^2(n(\Omega_{\vec{q}}) + \frac{1}{2} \mp \frac{1}{2})$$

where

$$J(\vec{q}) = \int e^{i\vec{q}\cdot\vec{r}} d\vec{r}$$

and $\vec{q}$ is a 3D wave vector.

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Figure Captions

Fig.1 Schematic diagram of the 3-band model used in the calculation for α_{ex}'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 $\alpha_{ex}^{(1)}$ for QWW as function of the photon energy $\hbar\omega$ at $L_x = L_y = 200A^\circ$ (solid curve) and at $Lx = Ly = 100A^\circ$ (dashed curve). we used the parameters characteristic of $Si_{0.5}Ge_{0.5}$: $m_e^* = 0.19m_0$, $m_h^* = 0.49m_0$, $Eg = 1.02eV, \hbar\Omega = 60$ meV, $E_{ex} = 10$ meV [Ref.14].

Fig.3 $\alpha_{ex}^{(2)}$ for layered QW as function of the photon energy $\hbar\omega$ at $L_z = 200A^\circ$ (solid line) and $L_z = 100A^\circ$ (dashed line) for the same compound.

Fig.4 $\alpha_{ex}^{(3)}$ for bulk case as function of the photon energy.

1D

First subband

Second subband

Phonon Absorption

Phonon Emission

$(E_G - \hbar\Omega - E^b_{ex})$

$(E_G + \hbar\Omega - E^b_{ex})$

$\alpha^{(1)}_{ex}(\omega)$ (arbitrary units)

1 2 3 4 5 6 7 8

0.94 0.99 1.04 1.09 1.14

$\hbar\omega$(eV)

Fig.2

2D

$\alpha^{(2)}_{ex}(\omega)$ (arbitrary units)

1 2 3 4 5 6 7 8

First Subband

Second Subband

Phonon Absorption

Phonon Emission

$(E_G - \hbar\Omega - E^b_{ex})$

$(E_G + \hbar\omega - E^b_{ex})$

0.92 0.97 1.02 1.07

$\hbar\omega$ (eV)

Fig.3

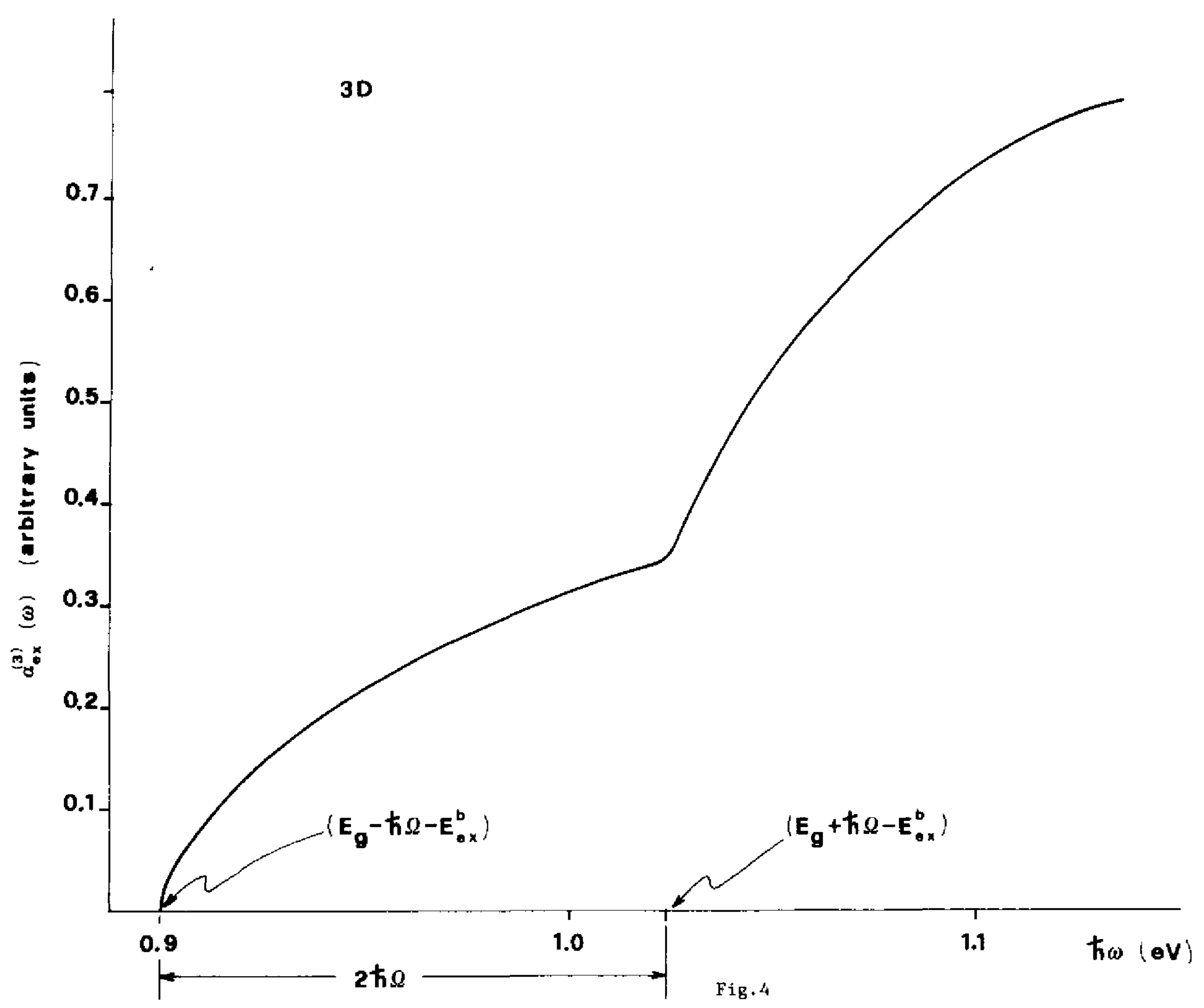

Fig.4