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Ideal interband absorption spectra in an indirect-gap-semiconductor quantum well

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We have derived the expression for an absorption coefficient in a quantum well made of an indirect-gap semiconductor, considering phonon-assisted and no-phonon (alloy-disorder) processes. The absorption coefficient varies as $(\hbar\omega_\lambda - E_g \pm \hbar\omega_p)^s$, where $\hbar\omega_\lambda$ $(\hbar\omega_p)$ is the photon (phonon) energy and E_g is the band gap; $s=0$ for bound excitonic absorption and $s=1$ for band-to-band or continuum-state transitions. For transitions to the excitonic continuum states, the absorption coefficient increases linearly for high values of photon energy.

I. INTRODUCTION

Interband optical absorption and emission processes in indirect-gap semiconductors like Si, Ge, and their alloys were studied quite thoroughly in the early days of semiconductor research.[1-4] However, attention was gradually shifted to direct-gap semiconductors[5,6] and later on, to the heterojunctions and quantum wells (QW's) made of them,[7,8] because of the suitability of these materials and their microstructures in optoelectronic device applications. The situation has changed somewhat only recently, since strained $\mathrm{Si}/\mathrm{Si}_x\mathrm{Ge}_{1-x}$ systems have shown promise for use in photonic devices.[9-14] The band gap in these indirect-gap QW's is compatible with the wavelengths for present day fiber-optic communication. Interband and intersubband absorption[13] in Si-SiGe QW's have already been investigated.

In spite of the recent intensive efforts in elucidating and exploiting the optical properties of indirect-gap QW's, some simple basic problems still remain unaddressed. It is well known[1-6] that the absorption coefficient in bulk indirect-gap materials varies as $(\hbar\omega_\lambda - E_g \pm \hbar\omega_p)^s$, where $\hbar\omega_\lambda$ $(\hbar\omega_p)$ is the photon (phonon) energy, E_g is the band gap, and the values of the exponent s are 2 and $\frac{1}{2}$, respectively, for simple band-to-band transitions and for bound excitonic absorption. No attempt has yet been made to examine how this exponent s changes in indirect-gap QW's. On the other hand, the absorption spectra in Si/(Si,Ge) QW's have been analyzed, on the assumption that the exponent $s=2$, in some recent work.[14]

The purpose of the present paper is to derive the expression for the absorption coefficient due to transitions from the valence band to the lowest indirect conduction-band subband in a QW. The transfer from the intermediate state to the final states occurs via phonon or alloy-disorder (no-phonon) scattering. The theory is outlined in Sec. II. The nature of the expected ideal (low-temperature) absorption spectra is discussed in Sec. III. Section IV gives the conclusion.

II. THEORY

The interband absorption in an indirect-gap semiconductor is a two-step process and the transition rate from an initial state $|i\rangle$ to the final state $|f\rangle$ via the intermediate states $|\mathrm{in}\rangle$ is given by the second-order perturbation theory as[15]

$$W = \frac{2\pi}{\hbar} \sum_f \left| \sum_{\mathrm{in}} \frac{\langle f|H|\mathrm{in}\rangle\langle \mathrm{in}|H|i\rangle}{E_i - E_{\mathrm{in}}} \right|^2 \delta(E_i - E_f) , \qquad (1)$$

where E is the energy, $H = H_\lambda + H_{ep}$, H_λ is the perturbation due to radiation field, and H_{ep} is the electron-phonon interaction potential. Using the above expression Ridley[15] has obtained the following for the transition rate:

$$W(\hbar\omega_\lambda) = \frac{V M_\lambda^2 D^2 g_v (m_c^* m_v^*)^{3/2}}{8\pi^2 (E_{g0} - \hbar\omega_\lambda)^2 \hbar^6 \rho \omega_p} \times [N_Q(\omega_p)(\hbar\omega_\lambda - E_g + \hbar\omega_p)^2 + \{N_Q(\omega_p)+1\}(\hbar\omega_\lambda - E_g - \hbar\omega_p)^2] . \qquad (2)$$

The absorption coefficient is given by

$$\alpha(\hbar\omega_\lambda) = W(\hbar\omega_\lambda)\eta / c . \qquad (3)$$

In the above, V is the crystal volume, M_λ is the matrix element for electron-photon interaction, D is the deformation-potential constant for electron-phonon interaction, g_v is the number of equivalent valleys for the final conduction-band state, m_c^* and m_v^* are the effective masses for electron (assumed isotropic) and for hole, respectively, E_{g0} (E_g) is the direct (indirect) band gap, ρ is the mass density, N_Q is the number of phonons with wave vector Q, $\hbar$ is reduced Planck constant, η is the refractive index of the material, and c is the velocity of light.

The QW is formed along the z direction. The transition is assumed to take place from an initial state $|vk\rangle$ in the valence subband of two-dimensional (2D) wave vector $\mathbf{k}$ to an intermediate state $|\Gamma k\rangle$ in the direct (zone center) conduction band and then to the final state $|ck'\rangle$ in the lowest conduction subband. The wave functions are given by

$$\begin{aligned} |vk\rangle &= u_v \exp(i\mathbf{k}\cdot\mathbf{r})\phi_{hl}(z) , \\ |\Gamma k\rangle &= u_\Gamma \exp(i\mathbf{k}\cdot\mathbf{r})\phi_\Gamma(z) , \qquad (4) \\ |ck'\rangle &= u_c \exp(i\mathbf{k}'\cdot\mathbf{r})\phi_{cm}(z) . \end{aligned}$$

In the above, ϕ's are envelope functions. ϕ_{hl} and ϕ_{cm}

denote confined states corresponding to subbands l and m. $|\Gamma k\rangle$ is a continuum state; however, the effective mass mismatch between the well and barrier materials gives rise to reflections at the boundaries of the well[16] and $\phi(z)$ is not as simple as $\exp(ik_z z)$. In the present derivation the detailed nature of ϕ's is not important, since the exact form is needed only when exact quantitative calculation is performed.

The matrix element for transition from the initial state to the intermediate state due to photon absorption is

$$M_\lambda^2=\left[\frac{eA_0}{m_0}\right]^2|\langle vk|\varepsilon_\lambda\cdot\mathbf{p}|\Gamma k\rangle|^2 , \tag{5}$$

where m_0 is the free-electron mass, ε_λ is the polarization vector of light wave, $\mathbf{p}$ is the momentum operator, and A_0 is the amplitude of the vector potential given by[17]

$$A_0^2=\frac{\hbar}{2\varepsilon_0\eta^2 V\omega_\lambda} \tag{6}$$

with ε_0 as the free space permittivity.

In the QW the matrix element depends on the angle between the polarization vector and the z axis.[18] Using Eq. (4) in Eq. (5), one obtains[18,19]

$$M_\lambda^2=\left[\frac{eA_0}{m_0}\right]^2\langle|p_{\Gamma v}|^2\rangle A_{l\Gamma}C_{l\Gamma} , \tag{7}$$

$$C_{l\Gamma}=\left|\int\phi_\Gamma(z)\phi_{hl}(z)dz\right|^2 . \tag{8}$$

$A_{l\Gamma}$ is the polarization-dependent part and $\langle|p_{\Gamma v}|^2\rangle$ is the average momentum matrix element.

The final state may be a simple electronic state or an excitonic state and the transition from the intermediate state to the final state may occur by phonon or alloy-disorder scattering. These different cases are considered below.

A. Interband transition: Nonexcitonic

The matrix element for transition from the intermediate state to the final state involving a phonon of energy $\hbar\omega_p$ may be written by extending Ridley's treatment[15] for bulk materials to the QW case. The interaction potential is assumed to be independent of the phonon wave vector $\mathbf{Q}$ $(\equiv\mathbf{q},q_z)$,[20] and thus

$$|\langle ck'|H_{ep}|\Gamma k\rangle|^2=\sum_{\mathbf{k}',q_z}\frac{\hbar D^2}{2\rho V\omega_p}(N_Q+\tfrac{1}{2}\mp\tfrac{1}{2})\times\delta_{\mathbf{k}\pm\mathbf{q},\mathbf{k}'}|I(q_z)|^2 , \tag{9}$$

where

$$|I(q_z)|^2=\left|\int_0^L\phi_\Gamma(z)e^{iq_z z}\phi_{cm}(z)dz\right|^2 \tag{10}$$

is the overlap integral for electron-phonon interaction.[21] The Kronecker δ indicates momentum conservation in the plane of the QW layer.

The expression for the transition probability becomes

$$W(\hbar\omega_\lambda)=\frac{2\pi}{\hbar}\left[\frac{eA_0}{m_0}\right]^2\frac{A_{l\Gamma}C_{l\Gamma}\langle|p_{\Gamma v}|^2\rangle}{(E_{g0}-\hbar\omega_\lambda)^2}\left[\frac{\hbar D^2}{2\rho V\omega_p}\right]\times\sum_{\mathbf{k},\mathbf{k}',q_z}(N_Q+\tfrac{1}{2}\mp\tfrac{1}{2})\delta(E_{\mathbf{k}'}-E_{\mathbf{k}}\mp\hbar\omega_p)\times|I(q_z)|^2 . \tag{11}$$

The summations over $\mathbf{k}$, $\mathbf{k}'$, and q_z are converted into integrals in the usual way. The summation over q_z is written as[21]

$$\sum|I(q_z)|^2=\frac{L}{2\pi}F(\Gamma,c) . \tag{12}$$

The form factor F has been worked out in the literature[21] for simple envelope functions. The summations over $\mathbf{k}$ and $\mathbf{k}'$ may be converted into the following integral:

$$J=\int\delta(E_{\mathbf{k}'}-E_{\mathbf{k}}\mp\hbar\omega_p)k'dk'd\theta'k\,dk\,d\theta . \tag{13}$$

Using parabolic dispersion relation, $E_{\mathbf{k}'}=E_g+\hbar^2k'^2/2m_c^*$, the k' integration is easily done by using the δ function, yielding a constant energy-independent factor. The integration over $\mathbf{k}$ is then converted to an integration over $E_k=\hbar^2k^2/2m_v^*$ with the limits 0 and $(\hbar\omega_\lambda-E_g\pm\hbar\omega_p)$. Collecting all the constant factors, taking a factor 2 for spin degeneracy and a term g_v for valley degeneracy, one obtains

$$\alpha(\hbar\omega_\lambda)=\frac{B_{bbph}}{\hbar\omega_\lambda}\frac{1}{L}(N_Q+\tfrac{1}{2}\mp\tfrac{1}{2})(\hbar\omega_\lambda-E_g\pm\hbar\omega_p)\times H(\hbar\omega_\lambda-E_g\pm\hbar\omega_p) , \tag{14}$$

where

$$B_{bbph}=\frac{e^2A_{l\Gamma}C_{l\Gamma}\langle|p_{\Gamma v}|^2\rangle D^2m_c^*m_v^*g_vF(\Gamma,c)}{8\pi^2m_0^2\varepsilon_0\eta\rho c\omega_p\hbar^2(E_{g0}-\hbar\omega_\lambda)^2} . \tag{15}$$

In the above $H(x)$ is a step function, and E_g is the effective band gap, i.e., the actual band gap plus the subband energies for an electron and a hole. The absorption coefficient in the above denotes the intensity reduction of light as it propagates through the QW layer plane.

B. Bound excitonic transition

The absorption due to transition from valence band to the bound excitonic states was treated by Elliott[1] and discussed in detail by several workers.[1-6] Following the treatment by McLean,[2] but changing the notations, we may write the absorption coefficient as

$$\alpha(\hbar\omega_\lambda)=\frac{B'_{bxph}}{\hbar\omega_\lambda}\sum_{n=1}^{\infty}|\psi_{nk_c}(0)|^2\times\sum_{\mathbf{K},q_z}\delta\left[E_g+\frac{\hbar^2K^2}{2M}-\frac{E_{\text{ex}}(\mathbf{k}_c)}{(n-\frac{1}{2})^2}\mp\hbar\omega_p-\hbar\omega_\lambda\right]\times(N_Q+\tfrac{1}{2}\mp\tfrac{1}{2}) , \tag{16}$$

$$\psi_{lk_c}(r)=\left[\frac{2}{\pi}\right]^{1/2}\frac{2}{a_B}\exp(-2r/a_B)\ , \tag{17}$$

$$|\psi_{nk_c}(r=0)|^2=\frac{1}{(2n-1)^3}|\psi_{1s}(r=0)|^2\ . \tag{18}$$

In the above ψ is the excitonic envelope function,[22] r is the separation of an electron and a hole in the plane, $\mathbf{k}_c$ is the location of conduction-band minima in $\mathbf{k}$ space, M is the total mass, and $\hbar\mathbf{K}$ is the center-of-mass momentum, E_{ex} is the exciton binding energy in the bulk material, and a_B is the bulk exciton Bohr radius. Converting summation into integration, one gets

$$\alpha(\hbar\omega_\lambda)=\frac{B_{bxph}}{\hbar\omega_\lambda}\frac{1}{L}\sum_{n=1}^{\infty}\frac{1}{(2n-1)^3}\times H\left[\hbar\omega_\lambda-E_g+\frac{E_{\mathrm{ex}}}{(n-\frac{1}{2})^2}\pm\hbar\omega_p\right]\times(N_Q+\tfrac{1}{2}\mp\tfrac{1}{2})\ , \tag{19}$$

where

$$B_{bxph}=\left[\frac{16M\hbar^2}{m_c^*m_v^*a_B^2}\right]B_{bbph}\ . \tag{20}$$

C. Transition to excitonic continuum states

For the unbound (continuum) states, one may use the approximate (2D) Sommerfeld factor[22]

$$|\psi_k(r=0)|^2=\frac{1}{1+\exp(-2\pi/a_Bk)}\ . \tag{21}$$

The absorption coefficient may be written as

$$\alpha(\hbar\omega_\lambda)=\frac{B'_{cxph}}{\hbar\omega_\lambda}\frac{1}{L}\int d^2K\int d^2k\,dq_z\frac{2}{1+\exp(-2\pi/a_Bk)}\times\delta\left[E_g+\frac{\hbar^2K^2}{2M}+\frac{\hbar^2k^2}{2\mu}\mp\hbar\omega_p-\hbar\omega_\lambda\right](N_Q+\tfrac{1}{2}\mp\tfrac{1}{2})\ . \tag{22}$$

Thus

$$\alpha(\hbar\omega_\lambda)=\mathcal{M}I_\pm(\hbar\omega_\lambda) \tag{23}$$

with

$$I_\pm(\hbar\omega_\lambda)=\int_0^{\sqrt{\Delta}}\frac{2k\,dk}{1+\exp(-2\pi/a_Bk)} \tag{24}$$

and

$$\Delta=\frac{2\mu}{\hbar^2}(\hbar\omega_\lambda-E_g\pm\hbar\omega_p)\ .$$

In the above $\mathcal{M}$ stands for "multiplying factor" and μ is the reduced mass. The above integral is evaluated numerically. However, when the upper limit is large, i.e., photon energy is large, it is easy to verify that the value of the integral approaches $(\hbar\omega_\lambda-E_g\pm\hbar\omega_p)$. The final expression is

$$\alpha(\hbar\omega_\lambda)=\frac{B_{cxph}}{\hbar\omega_\lambda}\frac{1}{L}(N_Q+\tfrac{1}{2}\mp\tfrac{1}{2})I_\pm(\hbar\omega_\lambda) \tag{25}$$

and

$$B_{cxph}=\left[\frac{M\hbar^2}{m_c^*m_v^*}\right]B_{bbph}\ . \tag{26}$$

D. No-phonon (alloy-disorder) process

The transition from the intermediate states to the final states near $\mathbf{k}=\mathbf{k}_c$ may occur via scattering by alloy-disorder potential.[3,4] The method to treat this case would be to replace the matrix element for phonon scattering given by Eq. (9) by the corresponding one for alloy-disorder scattering. We shall assume, following the theory for mobility in QW's due to alloy disorder,[23] that the scattering potential is a spherically symmetric square well of height ΔE and radius r_0 randomly distributed among the alloy sites in the alloy material A_xB_{1-x}. The matrix element for transition considering all the alloy sites is given by

$$|\langle\Gamma k|H_{\mathrm{alloy}}|ck'\rangle|^2=\left[\frac{4\pi}{3}r_0^3\right]^2\Delta E^2x(1-x)N_0\times\int|\phi_\Gamma(z)|^2|\phi_{cl}(z)|^2dz\ , \tag{27}$$

where N_0 is the total number of cation sites per unit volume. It is now straightforward to repeat the earlier calculation and quote the result for transition to exciton continuum as follows:

$$\alpha(\hbar\omega_\lambda)=\frac{B_{cxal}}{\hbar\omega_\lambda}\frac{1}{L}(\hbar\omega_\lambda-E_g)\ , \tag{28}$$

where

$$B_{cxal}=\left[\frac{64\pi^3}{9}\frac{x(1-x)N_0\rho\omega_pL^2\Delta E^2r_0^6I_0(\Gamma,c)}{\hbar D^2F(\Gamma,c)}\right]B_{bbph} \tag{29}$$

and

$$I_0(\Gamma,c)=\int|\phi_\Gamma(z)|^2|\phi_{cl}(z)|^2dz\ . \tag{30}$$

III. RESULTS AND DISCUSSIONS

The expressions derived in Sec. II can in principle be used to calculate the absorption coefficient in an indirect-gap QW, made of, e.g., $\mathrm{Si}_x\mathrm{Ge}_{1-x}$ or Si. However, the calculation is rather involved since most of the parameters are unknown even for bulk materials. The parameters in the strained system must be known as a function of composition x also. We shall therefore discuss some qualitative features of the absorption coefficient and restrict our attention to the ideal 0-K situation, with no broadening of the lines at all.

We present in Fig. 1 the variation of the function

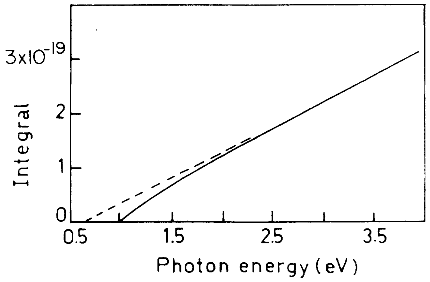

FIG. 1. Variation of the value of the integral defined by Eq. (24) in the text with photon energy. The value increases linearly (indicated by the dashed line) as the photon energy increases.

$I(\hbar\omega_\lambda)$ given by Eq. (24) as a function of photon energy $\hbar\omega_\lambda$. For numerical calculation, the parameters for $\mathrm{Si}_{0.5}\mathrm{Ge}_{0.5}$ are used:[9,24,25] $m_c^*=0.19m_0$, $m_v^*=0.49m_0$, $E_g=1.02$ eV, $\hbar\omega_p=60$ meV, $E_{\mathrm{ex}}=10$ meV. The curve indicates that near the threshold, i.e., $\hbar\omega_\lambda=E_g\pm\hbar\omega_p$, the function is superlinear; however, as expected, the curve is linear for larger values of $\hbar\omega_\lambda$. This trend has been predicted in Sec. II and agrees with the relation $(\hbar\omega_\lambda-E_g\pm\hbar\omega_p)^1$ obtained from Eq. (14). It should be noted that a similar trend is also found in bulk materials, where the absorption for transition to continuum states is given by $(\hbar\omega_\lambda-E_g\pm\hbar\omega_p)^2$ for large photon energy and agrees with the expression obtained for simple band-to-band transitions.

The expressions derived in Sec. II also give us the idea how α should vary in a QW. We display the expected variation for phonon-assisted processes in Fig. 2. The magnitude of the absorption, the locations of the steps and the breaks, and slopes of the curves are completely arbitrary. The curve is included only for illustration. We assume that only one type of phonon is involved and that its energy is in between the energies for second and third subbands.

At the threshold, there is a sharp rise of absorption due to transition to the 1s bound excitonic state attached to the first subband. There are a few more steps for higher bound states. The absorption then rises due to the involvement of the continuum states, and shows a linear increase given by $(\hbar\omega_\lambda-E_g+\hbar\omega_p)$. When transition to the bound exciton states attached to the second subband occurs, new steps come in, but the previous linear rise is also present. The absorption curve changes its slope, as the continuum states belonging to the second subbands are scanned. Finally a break occurs as the phonon emission process sets in. Additional structures are introduced when the photon energy is increased further so that the final states are in the third subband. The absorption curve becomes more complex due to the involvement of additional phonons and alloy-disorder scattering. The actual curve at finite temperatures should involve a convolution of the basic spectra with a line-shape function arising from fluctuation in well width, scattering processes, and finite temperature effects. The actual variation of absorption coefficient is difficult to predict. In some recent analyses[14] the experimental data on QW's are made to fit a $(\hbar\omega_\lambda-E_g)^2$ law valid for bulk $\mathrm{Si}_x\mathrm{Ge}_{1-x}$.

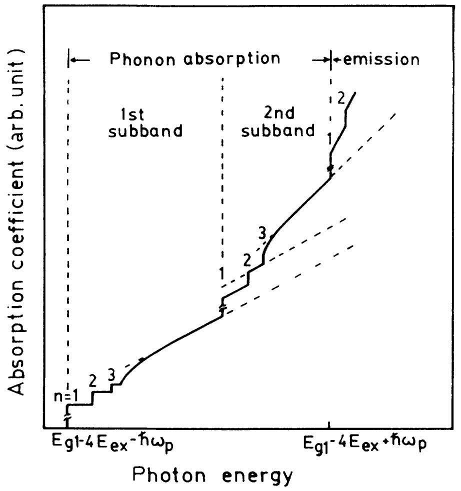

FIG. 2. Qualitative variation of the absorption coefficient with photon energy in the presence of a single intervalley phonon. The height of steps and the slopes of the curves are completely arbitrary. The locations of the steps are obtained from the Heaviside step function in Eq. (19) and n denotes excitonic state.

IV. CONCLUSIONS

The spectral dependence of the absorption in indirect-gap QW's is found from theoretical grounds to obey a law $(\hbar\omega_\lambda-E_g\pm\hbar\omega_p)^s$, where s takes a value 0 for bound excitonic transitions and a value 1 for band-to-band or continuum state transitions. The values of the exponent s are, respectively, $\frac{1}{2}$ and 2 in bulk materials.

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