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Optical absorption in semiconducting quantum-well structures: Indirect interband transitions

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The optical absorption in semiconducting quantum-well structures is calculated for the case where the quantum well consists of an indirect-band-gap semiconductor. The absorption is obtained for the cases where the carriers are confined in either quasi-one- or quasi-two-dimensional structures. The absorption is found to be a nonmonotonic function of the photon energy for a fixed width of the quantum well. However, the exact behavior of the absorption due to interband transitions between the valence and conduction bands of the semiconductor is different for quasi-one- and quasi-two-dimensional structures reflecting the different behavior of the density of states for carriers confined in such quasi-one- and quasi-two-dimensional structures. Our results for quasi-one- and quasi-two-dimensional systems converge to each other in the appropriate limits and also to the results obtained for an indirect-band-gap semiconductor in the bulk limit.

I. INTRODUCTION

With the steady improvement in molecular-beam epitaxy (MBE) and metal-organic chemical-vapor (MOCVD) techniques, it has become possible to fabricate sophisticated submicrometer devices whose dimensions are of the order of the thermal de Broglie wavelength of the charge carriers in such structures.[1–4] The optical and electrical transport properties of such quantum-well and superlattice structures have been the subject of much investigation, both theoretically[5–10] and experimentally.[2,3,11–15] Most of the recent work on quantum-well heterostructures and superlattices has been performed using GaAs/$\text{Ga}_{1-x}\text{Al}_x\text{As}$ systems, where GaAs is a direct-band-gap semiconductor, although work has been done on InAs/GaSb and Hg-CdTe systems.[16,17] More recently, work has been done by fabricating superlattice systems of amorphous silicon[18,19] and some of the optical and electrical properties of this system have been studied experimentally. Since silicon is an indirect-band-gap semiconductor, its optical properties are different from GaAs since in the former material, interband transitions between the valence and conduction bands of the semiconductor can only take place via a process in which the carriers are simultaneously scattered by lattice imperfections such as phonons when they absorb light.[20] In addition, there are other potential semiconducting quantum-well systems which are of some interest such as those involving GaP or Ge (Ref. 21) in which an important component of the system is an indirect-band-gap semiconductor. In fact, in a detailed treatment of GaAs/$\text{Ga}_{1-x}\text{Al}_x\text{As}$ quantum-well systems, one has to take account of the fact that GaAs has a higher band with an indirect band gap of 1.8 eV.[22] Therefore, it is important to extend previous treatments of the optical properties of semiconducting quantum-well systems[2] to the case where the semiconductor has an indirect band gap.

In this paper we calculate the interband optical absorption for a semiconducting quantum well system where the active semiconducting layer is made of a material having an indirect band gap. Since such quantum-well systems have been fabricated which are not only quasi-two-dimensional in their nature because of the confinement of the carriers in a layer structure but have also been fabricated in the form of quantum-well wires[23] where the carriers behave as a quasi-one-dimensional electron gas, we will consider both quasi-one- and quasi-two-dimensional quantum-well structures. The optical absorption in quantum-well wires fabricated from direct-band-gap semiconducting materials has been theoretically calculated.[24] In our calculations, we will use a parabolic two-band model for the conduction and valence bands of the semiconductor where the maximum in the valence band occurs at a different point in k space than the minima in the conduction band. In our model we will assume that the confining potential barrier can be approximated by an infinite square-well potential. This approximation will be fairly good if we are studying transitions between the states which lie close to the bottom of the potential well although it will break down for very narrow potential wells where the lowest-energy levels lie close to the top of the potential well. Even for the more general case, the use of the infinite potential-well model should yield results which are qualitatively, if not quantitatively, close to what one would expect to observe experimentally.

In Sec. II the theoretical results of our calculations are presented together with the model and the various approximations we have used. We consider indirect transitions in which the electron in the valence band absorbs a photon and is simultaneously scattered by the emission or absorption of a phonon. In our treatment we will consider interactions with acoustic phonons and with both polar and nonpolar optical phonons. The interaction with nonpolar optical phonons should be important in nonpolar materials such as silicon or germanium, while the interaction with polar optical phonons will play an important role in weakly ionic semiconductors such as the III-V semiconducting compounds. In Sec. III we will present our numerical results and discuss their relevance to possible experiments.

II. THEORY

The model we use in our calculations of the interband optical absorption in indirect-band-gap semiconducting quantum-well structures is similar to that presented by Smith[25] for bulk semiconductors. In this model we assume conduction and valence bands which are parabolic in the vicinity of the band extrema with the maximum in the valence band and the minimum in the conduction band occurring at different points in k space. We assume an isotropic effective mass for the electron in the vicinity of the band extrema with the maximum in the valence band occurring at $k=0$ and with M conduction-band minima, each a distance $\mathbf{k}_0$ from the valence-band maximum in k space. The indirect band gap E_g' in the semiconductor is less than the direct band gap E_g. Therefore, when the photon energy $\hbar\Omega$ is less than the direct band gap but greater than the indirect band gap, optical transitions can only occur when the electron gains the necessary momentum to make a transition from a state in the vicinity of the valence-band maximum to a state in the vicinity of one of the conduction-band minima by absorbing or emitting a phonon of wave vector whose magnitude is of order k_0. This is because the photon carries negligible momentum compared to the separation between the conduction- and valence-band extrema in k space. To calculate the probability of these phonon-assisted optical transitions we need to use second-order perturbation theory,[20,25] and obtain the following for the transition probability for this process:

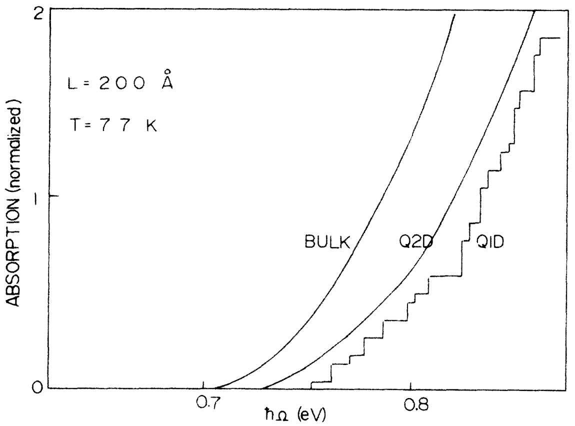

FIG. 1. The normalized optical absorption in an indirect-band-gap semiconductor is shown as a function of photon energy $\hbar\Omega$ in a quantum-well wire and a quasi-two-dimensional layered quantum-well structure for well widths of 200 Å at 77 K. The absorption is also shown for a bulk semiconductor of the same material parameters and with the same normalization coefficient. The parameters used in the calculation are of those of Ge.

$$W=(2\pi/\hbar)\sum_{k'n'}\left[\sum_{k''n''}\left|\frac{(k'n'\,|\,H_{\mathrm{rad}}\,|\,k''n'')(k''n''\,|\,V_s\,|\,kn)}{E_{k'n'}-E_{k''n''}+\hbar\omega}+\frac{(k'n'\,|\,V_s\,|\,k''n'')(k''n''\,|\,H_{\mathrm{rad}}\,|\,kn)}{E_{k''n''}-E_{kn}-\hbar\Omega}\right|\right]^2 . \tag{1}$$

In Eq. (1) the interaction Hamiltonians between the electrons and the radiation field H_{rad} and the phonon field V_s are given by

$$H_{\mathrm{rad}}=(-e/mc)\mathbf{A}\cdot\mathbf{p} \tag{2}$$

and

$$V_s(\mathbf{r})=\sum_{\mathbf{q}} C(\mathbf{q})[Q_q\exp(i\mathbf{q}\cdot\mathbf{r})+Q_{-q}^{\dagger}\exp(-i\mathbf{q}\cdot\mathbf{r})] . \tag{3}$$

Here, $C(\mathbf{q})$ is the wave-vector-dependent coupling coefficient between the electrons and the phonons and $Q_q,Q_{-q}^{\dagger}$ are the phonon creation and annihilation operators. For coupling to acoustic phonons, the coupling coefficient is

$$C(\mathbf{q})=iqE_d^{\mathrm{ac}}/(\rho V_0)^{1/2} ; \tag{4a}$$

for coupling to nonpolar optical phonons, the coupling coefficient is

$$C(\mathbf{q})=(\hbar/2\rho V_0)^{1/2}E_d^{\mathrm{op}} , \tag{4b}$$

while for coupling to polar optical phonons, it is

$$C(\mathbf{q})=ie\omega_0(4\pi/V_0\epsilon')^{1/2}\mathbf{q}\hat{\epsilon}_{\mathbf{q}}/q^2 . \tag{4c}$$

Here $E_d^{\mathrm{ac,op}}$ is the deformation potential constant for the semiconductor for coupling to either acoustic or optical phonons, ρ is the density of the material, ω_0 is the optical phonon frequency, and $1/\epsilon'=1/\epsilon_\infty-1/\epsilon_0$ where ϵ_∞ is the high-frequency dielectric constant and ϵ_0 is the static dielectric constant of the material.

For electrons confined in a quantum-well structure, we assume a model in which the confinement is in an infinite potential well. Although in realistic situations the potential well is finite, the use of the infinite-well model should yield good results if we are interested in transitions between subbands near the top of the valence band and the bottom of the conduction band. Using this model, the wave functions and energy eigenvalues for electrons and holes confined in quasi-one-dimensional quantum-well wire structures are

$$\psi(\mathbf{r})=(2/V_0^{1/2})u_\alpha(\mathbf{r})\sin(n_\alpha\pi x/a)\sin(l_\alpha\pi y)\exp(ik_\alpha z) , \tag{5}$$

$$E(n_c,l_c,k)=E_c+(\hbar^2k^2/2m_c)+n_c^2E_{ca}+l_c^2E_{cb} , \tag{6}$$

and

$$E(n_v,l_v,k_z)=E_v-(\hbar^2k^2/2m_v)-n_v^2E_{va}-l_v^2E_{vb} , \tag{7}$$

respectively, where E_c is the energy at the bottom of the conduction band, E_v is the energy at the top of the valence band, $k=k_z-k_0$, where k_0 is the location of the conduction-band minimum in k space,

$$E_{\alpha a(b)}=(\pi^2\hbar^2/2m_\alpha a^2[b^2]) ,$$

a and b are the sides of the quantum-well wire of rectangular cross section, the axis of the wire is taken to be the z direction, and m_α is the effective mass of the αth particle. Similarly, for electrons and holes confined in a quasi-two-dimensional well structure of width d, the wave function and eigenvalues are

$$\psi(\mathbf{r})=(2/V_0)^{1/2}u_\alpha(\mathbf{r})\sin(n_\alpha \pi z/d)\exp i(k_x x+k_y y) , \tag{8}$$

$$E(n_c,k-k_0)=E_c+\hbar^2(\mathbf{k}-\mathbf{k}_0)^2/2m_c+n_c^2E_{cd} , \tag{9}$$

and

$$E(n_v,k)=E_v-(\hbar^2k^2)/2m_v-n_v^2E_{vd} , \tag{10}$$

where $E_{\alpha d}=(\pi^2\hbar^2)/2m_\alpha d^2$. In the above, $u_\alpha(\mathbf{r})$ are the Bloch functions at the band edges of the conduction and valence bands and the direction of confinement is taken to be the z direction. Also, in Eq. (9) and (10), $\mathbf{k}$ and $\mathbf{k}_0$ are the components of these wave vectors in the plane of the quantum well.

Using the eigenfunctions and eigenvalues given by Eqs. (5)–(10) together with Eqs. (1)–(3), we find, using a straightforward approach such as that used by Smith,[25] the following expression for the absorption coefficient:

$$\alpha^{\pm}=[16\pi^2Me^2/ncm^2\Omega(E_g-\hbar\Omega)^2]\,|\mathbf{p}_{cv}\cdot\hat{\boldsymbol{\epsilon}}|^2 \times|C(k_0)|^2(n_{\mathbf{k}_0}+\tfrac{1}{2}\pm\tfrac{1}{2})J_N(E_m) . \tag{11}$$

Here the ± sign indicates processes which involve the emission and absorption of a phonon, respectively, n is the index of refraction of the semiconductor, n_{k0} is the Bose-Einstein distribution function for phonons of wave vector $\mathbf{k}_0$, where $\mathbf{k}_0$ is the wave vector necessary to bridge the separation in wave-vector space between the conduction-band minima and the valence-band maximum, $\mathbf{p}_{cv}$ is the matrix element of the momentum operator between the band-edge Bloch function $u_\alpha(\mathbf{r})$ for the conduction and valence bands, E_g and E_g' are the direct and indirect band gaps in the semiconductor, respectively, and

$$E_m=\hbar\Omega-E_g'\pm\hbar\omega_0 . \tag{12}$$

The quantity $J_N(E_m)$ is the convolution integral of the product of the density of states for the electrons in the conduction and valence bands for the quasi-N-dimensional structure

$$J_N(E)=\int_0^{E_m}dE\,N_v(E)N_c(E_m-E) , \tag{13}$$

and is given by

$$J_1(E_m)=(2\pi\hbar^2A^2)^{-1}(m_cm_v)^{1/2}\sum_{n_v,l_v,n_c,l_c}\Theta(E_m-(n_v^2+l_v^2)E_{0v}-(n_c^2+l_c^2)E_{0c}) \tag{14}$$

for a quasi-one-dimensional quantum-well structure, by

$$J_2(E_m)=m_cm_v/(2\pi\hbar^2L)^2\sum_{n_v,n_c}(E_m-n_v^2E_{0v}-n_c^2E_{0c})\Theta(E_m-n_v^2E_{0v}-n_c^2E_{0c}) \tag{15}$$

for a quasi-two-dimensional quantum-well structure and by

$$J_3(E_m)=(m_cm_v/\hbar^4)^{3/2}E_m^2/(16\pi^3) \tag{16}$$

in a bulk three-dimensional structure. In the above, A is the cross-sectional area of the quantum-well wire and L is the width of the quasi-two-dimensional quantum well. Also $\Theta(x)$ is the step function, i.e.,

$$\Theta(x)=\begin{cases}1, & x>0\\ 0, & x<0\end{cases} \tag{17}$$

and $N_c(E)$ and $N_v(E)$ are the density of states of the electrons in the conduction band and the holes in the valence band. From Eq. (11) together with Eqs. (14)–(16), we can find the dependence of the absorption coefficient on the photon energy, the indirect band gap and the temperature. The dependence of the absorption on the photon energy in an indirect-band-gap semiconductor depends on the dimensionality of the electron gas, being a quadratic function of the photon energy in a bulk semiconductor, a series of linear functions of the photon energy in a quasi-two-dimensional structure and a step function of the photon energy in a quasi-one-dimensional structure. The behavior of the absorption in a quantum-well wire for indirect interband transitions is similar to that found in a bulk indirect-band-gap semiconductor in the presence of a strong magnetic field.[26] This is because a strong magnetic field also constrains the electrons and holes to behave as a quasi-one-dimensional system. The quasi-two-dimensional expression for $J_N(E_m)$ can be obtained by replacing the summations over l_c and l_v in Eq. (14) by integrals over these quantum numbers while the bulk expression can be obtained by replacing the summations over n_c and n_v in Eq. (15) by integrals. Thus our results for quasi-one- and quasi-two-dimensional systems converge to each other in the appropriate limits and also to the results obtained for an indirect-band-gap semiconductor in the bulk limit.

III. NUMERICAL RESULTS AND DISCUSSION

In Figs. 1 and 2 the normalized absorption coefficient is shown as a function of photon energy at 77 and 300 K in a quantum-well wire and a layered quasi-two-dimensional quantum-well structure for wire thickness or layer width of 200 Å with the absorption in the bulk shown for comparison. The same normalization coefficient is used in both cases. The parameters used in these calculations are those characteristic of germanium with direct and indirect band gaps being taken as 0.88 and 0.73 eV at 77 K and as 0.81 and 0.66 eV at 300 K.[27] The electron and holes masses used in the calculation are $0.04m_0$ and $0.3m_0$, respectively,[28] where m_0 is the free-electron mass. The

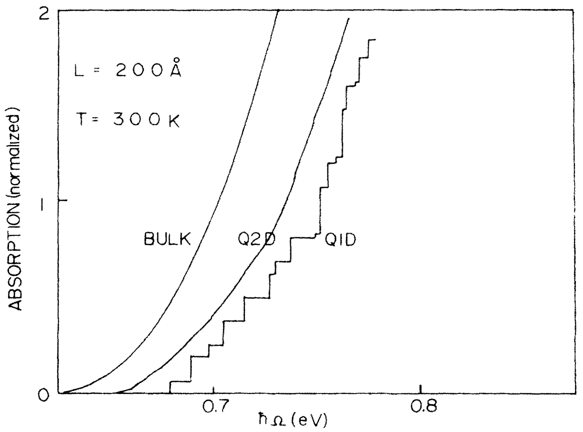

FIG. 2. The normalized optical absorption coefficient is shown as a function of photon energy at 300 K for the same cases and material parameters used in Fig. 1.

interband absorption is lower in a quasi-two-dimensional quantum-well structure than it is in the bulk and increases towards its bulk value as the dimensions of the quantum well increases. Also, the interband absorption is lower in a quantum-well wire than it is in a layered quantum-well structure, but again approaches its value in the bulk as the thickness of the wire increases. For a quasi-two-dimensional quantum-well structure, it can be seen that the absorption consists of a series of linear functions of the photon energy with changes in the slope of the absorption with photon energy whenever phonon-assisted transitions can occur between different sets of subbands in the conduction and valence bands. The behavior of the absorption here is similar to that predicted in direct-band-gap semiconductors for forbidden transitions.[24] For the case of a quantum-well wire, the absorption consists of a series of steps as a function of the photon energy with a new step occurring 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. In the figures it is being assumed that the main scattering is due to optical phonons where the energy of the optical phonons is 36 meV. Therefore, for a transition between a given set of subbands, there are two closely-lying steps which are separated in energy by 72 meV. The threshold for interband absorption to occur is shifted to higher photon energies from the bulk because of the increase of the effective band gap with the size quantization of the electronic energy levels.[24] The steps in the absorption due to processes in which phonons are absorbed increase dramatically as the temperature increases from 77 to 300 K. This reflects the increase in the number of phonons of wave vector $\mathbf{k}_0$ which are necessary for the phonon-assisted transitions with temperature. At high temperatures, transitions can occur with both emission and absorption of phonons while at low temperatures, where there are few phonons available of the wave vector needed for the phonon-assisted transitions, transitions can only occur with the emission of a phonon.

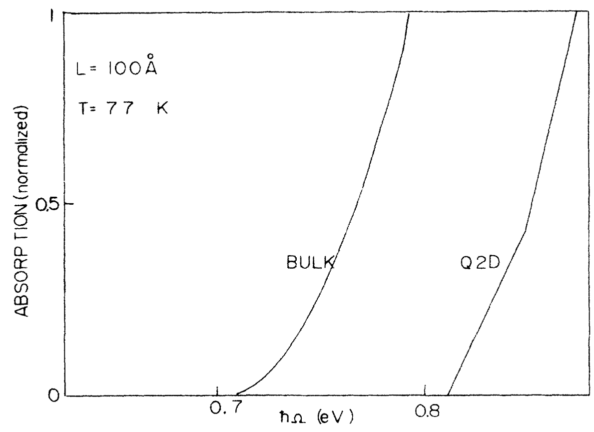

FIG. 3. The normalized optical absorption is shown as a function of photon energy for a layered quantum-well structure of width 100 Å and for a bulk semiconductor at 77 K. The same values of the material parameters are used as in Figs. 1 and 2.

In Figs. 3 and 4 the normalized absorption coefficient is shown as a function of the photon energy at 77 and 300 K for a quasi-two-dimensional quantum-well structure of width 100 Å with the bulk value also shown for comparison, and the parameters used in the calculation are again those characteristic of Ge. The normalization coefficient is the same as used in Figs. 1 and 2. Here, again the absorption is smaller in the quantum-well structure than it is in the bulk, with the absorption increasing as the well width increases. For this well width, the threshold for absorption in a quantum-well wire is shifted towards photon energies lying near the direct band gap of Ge, and therefore the results for a quantum-well wire are not shown for this wire thickness.

Our theoretical calculations show that for indirect-band-gap semiconducting quantum-well systems, the in-

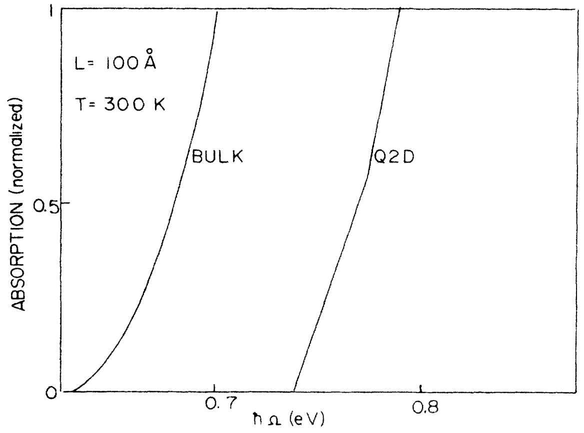

FIG. 4. The normalized optical absorption is shown as a function of the photon energy for the same cases as considered in Fig. 3 but at a temperature of 300 K.

terband optical absorption is smaller than in the bulk. The absorption is not as dramatic a function of the photon energy in quasi-two-dimensional semiconducting structures as it is for a direct-band-gap material where the absorption consists of a series of steps with increasing photon energy. The reason for the less dramatic dependence of the absorption on the photon energy in an indirect-band-gap semiconductor has to do with the fact that it depends upon the convolution of the electron and hole densities of states which washes out some of the sharp peaks and steps which occur in the absorption for quasi-one- and quasi-two-dimensional direct-band-gap semiconducting quantum-well structures. As mentioned earlier, similar effects occur in direct-band semiconducting quantum-well systems for forbidden transitions.[24] The temperature dependence of the absorption comes directly from the temperature dependences of the population of phonons of wave vector $\mathbf{k}_0$ which are involved in the phonon-assisted transitions between the top of the valence band and the bottom of the conduction bands.

Recently, the optical absorption has been studied in superlattice structures made from indirect-band-gap semiconductors such as GaP-GaAs$_x$P$_{1-x}$.[29] In these superlattice structures, the absorption was found to be enhanced over that observed in bulk samples of the indirect-band-gap semiconductors. This is different from the decreased absorption predicted in quantum-well structures made of indirect-band-gap semiconducting materials. However, these structures are not the same as the quantum-well structures considered in this paper, because the artificial periodicity introduced along the direction of confinement in superlattice structures introduces zero-folding effects which lead to the appearance of direct band gaps in the superlattice structure.[30–32] As a result of the appearance of these direct gaps, interband absorption can occur without phonon assistance in these multilayered superlattice structures, and therefore the absorption can be much larger than in the bulk material where phonons are needed for the interband absorption. In contrast, for a single quantum-well structure, which we have considered here, such zone-folding effects should not take place, and therefore the absorption should decrease over its value in the bulk.

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