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Free-carrier absorption in quasi-two-dimensional semiconducting structures

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The quantum theory of free-carrier absorption in semiconductors is extended to treat the case where the free carriers are confined in quasi-two-dimensional semiconducting structures such as layered heterojunctions, thin films, and inversion layers. As a result of the confinement of the carriers, the energy of motion of the carriers normal to the quasi-two-dimensional structure is size quantized. The free-carrier absorption coefficient is found to depend upon the polarization of the electromagnetic radiation relative to the direction normal to the quasi-two-dimensional structure and to be an oscillatory function of the thickness of the layer or film as a result of the size quantization. The free-carrier absorption coefficient is calculated for the case where the carriers are scattered by acoustic phonons via deformation-potential coupling.

I. INTRODUCTION

In recent years, there has been a growing interest in the electronic and optical properties of semiconducting layered heterojunctions,[1,2] thin films,[3–6] and inversion layers.[7–9] Because of the confinement of the carriers in these quasi-two-dimensional structures, size quantization begins to play an important role in determining their electrical and optical properties. Dingle[1] has reviewed the early work on the effects of size quantization on the optical absorption which occurs via interband transitions. Salpathy and Altarelli[10] have done some model calculations of the optical properties of quantum wells taking excitonic effects into account. Similar calculations of intersubband optical transitions have been performed by Hyzhnyakov *et al.*[11] and Bastard.[12] Holonyak and co-workers[13–15] have studied both theoretically and experimentally the optical emission from quantum wells because such quantum-well devices seem to hold great potential for use in lasers.[16] Voisin *et al.*[17] have also studied luminescence from quantum wells.

In addition to direct interband and intersubband optical transitions, optical absorption can take place via indirect intraband optical transitions in which the carriers absorb or emit a photon while simultaneously scattering off phonons or other imperfections in a crystal. Such free-carrier absorption accounts for the absorption of electromagnetic radiation of frequencies Ω lower than those which give rise to interband transitions in semiconductors, i.e., $\hbar\Omega < E_g$, where E_g is the band gap. The quantum theory of free-carrier absorption in bulk semiconductors was worked out by Meyer[18] and Rosenberg and Lax.[19] This theory was extended to take account of the presence of quantizing magnetic fields by several authors including ourselves[20–28] when the carriers were scattered by ionized impurities, optical phonons, and acoustic phonons. In quantizing magnetic fields, the motion of the carriers is also confined in the plane perpendicular to the magnetic field direction and it was found that the free-carrier absorption coefficient depended upon the polarization of the radiation field relative to the direction of the magnetic field.[27] For carriers confined in a quasi-two-dimensional structure, free-carrier absorption should be particularly important in determining the optical absorption when the carriers are confined to the lowest subband and the energy of the photon is insufficient to cause a transition to the next higher subband.

In this paper, we extend the quantum theory of the free-carrier absorption in semiconductors previously developed[18,19,25–28] to take account of the quantization of the energy levels of carriers which are confined by their motion in quasi-two-dimensional semiconducting structures. We consider the free-carrier absorption for the cases where the radiation field is polarized in the plane of the layer or film. Only the case where the carriers are scattered by their interaction with acoustic phonons via the deformation-potential coupling mechanism will be considered in this paper, because the calculation of the absorption coefficient is much simpler in this case than for the cases where ionized impurity scattering or polar optical-phonon scattering are important. The results obtained for acoustic-phonon

scattering can easily be extended to the case where nonpolar optical-phonon scattering may be important[26] such as may be the case in thin films or inversion layers of silicon. Finally, the size dependence of the free-carrier absorption coefficient will be explained in Sec. III in terms of the size dependence of the scattering rates and the possibility of phonon-assisted transitions between the various size-quantized subbands of the quasi-two-dimensional structure.

II. FREE-CARRIER ABSORPTION OF CONFINED CARRIERS

The absorption coefficient K for free-carrier absorption can be related to the quantum-mechanical transition probabilities for the absorption and emission of photons[18,25]

$$K=\frac{\epsilon^{1/2}}{n_0 c}\sum_i (W_i^{\rm abs}-W_i^{\rm em})f_i \ , \tag{1}$$

where ϵ is the dielectric constant of the material, n_0 is the number of photons in the radiation field, and f_i is the free-carrier distribution function. The sum goes over all the initial states i of the system. The transition probabilities $W_i^{\rm abs,em}$ can be calculated using the Born, second-order Golden Rule approximation

$$W_i^{\rm abs,em}=\frac{2\pi}{\hbar}\sum_f |(f\,|\,M\,|\,i)|^2 \times\delta(E_f-E_i\mp\hbar\Omega\pm\hbar\omega_q) \ , \tag{2}$$

where $(f\,|\,M\,|\,i)$ are the transition-matrix elements for this interaction

$$(f\,|\,M\,|\,i)=\sum_n\left[\frac{(f\,|\,H_{\rm rad}\,|\,n)(n\,|\,V_s\,|\,i)}{E_i-E_n\mp\hbar\omega_q}+\frac{(f\,|\,V_s\,|\,n)(n\,|\,H_{\rm rad}\,|\,i)}{E_i-E_n\pm\hbar\Omega}\right] . \tag{3}$$

Here E_f and E_i are the initial and final energies of the electron, $H_{\rm rad}$ is the interaction Hamiltonian between the electrons and the radiation field, V_s is the scattering potential due to the electron-phonon interaction, and $\hbar\Omega$ and $\hbar\omega_q$ are the energies of the photon and phonon, respectively. The sum is over all the intermediate states n of the system. The above expressions have to be evaluated using the energy eigenfunctions and eigenvalues of the free carriers. For electrons confined to move in the x-y plane in a semiconductor having parabolic energy bands, the eigenvalues and eigenfunctions are

$$E_{kn}=n^2E_0+\frac{\hbar^2k^2}{2m^*} \ , \quad E_0=\pi^2\hbar^2/2m^*d^2 \ , \quad n=1,2,3,\ldots \tag{4}$$

$$\psi(\vec{r},z)=\left[\frac{2}{\Omega_0}\right]^{1/2}\exp(i\,\vec{k}\cdot\vec{r})\sin(n\pi z/d) \ , \tag{5}$$

where Ω_0 is the volume of the material, d is the thickness of the film or layer, $\vec{k}$ is the carrier wave vector in the x-y plane, $\vec{r}$ is the position vector in this plane, and m^* is the effective mass of the carriers.

The matrix elements of the electron-phonon and electron-photon interaction Hamiltonians using the wave functions are

$$(\alpha'\,|\,V_s\,|\,\alpha)=\frac{1}{2}\left[\frac{k_BT}{2\rho u^2\Omega_0}\right]^{1/2}E_d\delta_{k_x',k_x+q_x}\delta_{k_y',k_y+q_y} \times(\delta_{q_z,(\pi/d)(n'-n)}+\delta_{q_z,-(\pi/d)(n'-n)}-\delta_{q_z,(\pi/d)(n'+n)}-\delta_{q_z,-(\pi/d)(n'+n)}) \tag{6}$$

and

$$(\alpha'\,|\,H_{\rm rad}\,|\,\alpha)=-\frac{e\hbar}{m^*}\left[\frac{2\pi\hbar n_0}{\epsilon\Omega\Omega_0}\right]^{1/2}\hat{\epsilon}\cdot\vec{k}\,\delta_{n',n}\delta_{k_x',k_x}\delta_{k_y',k_y} \ , \tag{7}$$

when the radiation field is polarized in the plane of the layer and

$$(\alpha'\,|\,H_{\rm rad}\,|\,\alpha)=\frac{-ie\hbar}{m^*}\left[\frac{2\pi\hbar n_0}{\epsilon\Omega\Omega_0}\right]^{1/2}\frac{n}{d}\left[\frac{1-\cos[\pi(n'-n)]}{n'-n}+\frac{1-\cos[\pi(n'+n)]}{n'+n}\right]\delta_{k_x',k_x}\delta_{k_y',k_y} \ , \tag{8}$$

when the radiation field is polarized perpendicular to the plane of the layer. Here ρ is the density of the semi-

conductor, u the sound velocity, and E_d is the deformation potential. When these matrix elements, together with the distribution function for a quasi-two-dimensional nondegenerate electron gas,

$$f_{kn}=\left[\frac{2\pi\hbar^2 n_e d}{m^* k_B T\gamma}\right]\exp\left[-n^2\frac{E_0}{k_B T}\right]\exp\left[-\frac{\hbar^2 k^2}{2m^* k_B T}\right],\quad \gamma=\sum_{n=1}^{\infty}\exp\left[\frac{-n^2 E_0}{k_B T}\right], \tag{9}$$

are used in Eqs. (1)—(3), we obtain the free-carrier absorption coefficient for a quasi-two-dimensional electron gas for radiation polarized in the plane of the film or layer

$$K=\frac{2\pi e^2(k_B T)^2 n_e E_d^2}{\hbar^4 c\rho u^2\Omega^3 d\gamma\epsilon^{1/2}}\sum_{n_i=1}^{\infty}\sum_{n_f=1}^{N_f}(1+\tfrac{1}{2}\delta_{n_f,n_i})\exp\left[\frac{-n_i^2 E_0}{k_B T}\right]\times\left[1+\frac{\hbar\Omega-(n_f^2-n_i^2)E_0}{2k_B T}\right]\left[1-\exp\left[-\frac{\hbar\Omega}{K_B T}\right]\right], \tag{10}$$

where N_f is the largest integer equal to or less than $(n_i^2+\hbar\Omega/E_0)^{1/2}$.

Here n_e is the carrier density per unit volume. For comparison, the free-carrier absorption in a nondegenerate bulk semiconductor is[25]

$$K_b=\frac{2}{3}\left[\frac{n_e e^2 E_d^2}{\rho u^2\hbar^3 c\Omega}\right]\left[\frac{2m^* k_B T}{\pi\epsilon}\right]^{1/2}\times\exp\left[\frac{\hbar\Omega}{2k_B T}\right]K_2\left[\frac{\hbar\Omega}{2k_B T}\right]\times\left[1-\exp\left[-\frac{\hbar\Omega}{k_B T}\right]\right], \tag{11}$$

where $K_n(x)$ is a modified Bessel function of the second kind. In the quantum limit, in which only the $n_i=1$ (ground) quantum level is occupied, the ratio of the free-carrier absorption in a quasi-two-dimensional system to that in the bulk

$$\frac{K}{k_b}=\frac{3\pi^{1/2}(k_B T)^{3/2}E_0^{1/2}}{(\hbar\Omega)^2 K_2\left[\frac{\hbar\Omega}{2k_B T}\right]}\times\sum_{n=1}^{N}\exp\left[\frac{\hbar\Omega}{2k_B T}\right](1+\tfrac{1}{2}\delta_{n,1})\times\left[1+\frac{\hbar\Omega-(n^2-1)E_0}{2k_B T}\right], \tag{12}$$

where N is the largest integer which is less than or equal to $(1+\hbar\Omega/E_0)^{1/2}$. In Fig. 1, the normalized free-carrier absorption coefficient,

$$K_N=(K/K_b)[(\hbar\Omega/k_B T)^{3/2}/3\pi^{1/2}]\times\exp(\hbar\Omega/2k_B T)K_2(\hbar\Omega/2k_B T),$$

is shown as a function of d^{-1}, where the parameter x is defined as

$$x^2=E_0/\hbar\Omega=\pi^2\hbar/2m\Omega d^2 .$$

The parameters used in the calculations leading to Fig. 1 are those characteristic of InSb with a carrier effective mass $m^*=0.013m_0$, where m_0 is the free-electron mass, at a temperature of 30 K and in a radiation field of wavelength 10 μm characteristic of a CO_2 laser. The ratio of the absorption coefficient in a quasi-two-dimensional structure to the bulk is a function of two dimensionless parameters, $E_0/\hbar\Omega$ and $\hbar\Omega/k_B T$ so that the results presented in Fig. 1 can be scaled to other materials by changing the temperature, photon frequency, and layer thickness. For small x, which corresponds to large width d of the layer, the free-carrier absorption coefficient is an oscillatory function of d^{-1} while for large x, the absorption coefficient increases linearly with d^{-1}. Therefore, for very narrow layers, the free-carrier absorption increases as the width of the layer decreases. There is an inflection point in the absorption coefficient as a function of d^{-1} whenever the photon energy is such that a phonon-assisted transition can take place to one of the higher subbands of the quantum well. The peaks in the absorption occur at values of x which are slightly smaller than those at which the inflection points occur. The absorption coefficient should show similar oscillatory behavior as a function of photon frequency for fixed width of the quantum well.

When the doping level of the well is high enough so that the free carriers are degenerate, the electron-distribution function for the quasi-two-dimensional electron gas is

$$f_{kn}=\begin{cases}1, & E_f<E_{kn}\\ 0, & E_f>E_{kn}\end{cases} \tag{13}$$

where the Fermi energy of the carriers is

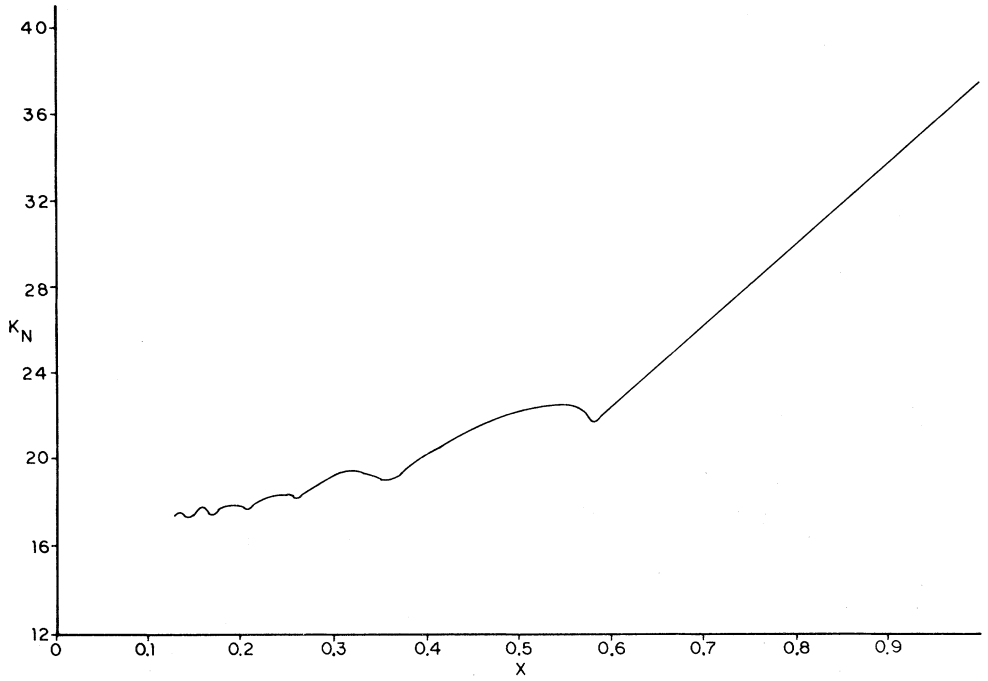

FIG. 1. The normalized free-carrier absorption coefficient is shown as a function of x where x measures the reciprocal of the layer width, d, in normalized units. The parameters used are those characteristic of n-type InSb at 30 K in a radiation field of 10 μm wavelength.

$$E_f = 2\pi\hbar n_e d/m^* .$$

Using this distribution function in Eqs. (1)—(3), we obtain for the free-carrier absorption coefficient for a quasi-two-dimensional degenerate electron gas the expression

$$K = \frac{e^2 k_B T E_d^2}{16 m^* \hbar^2 c \epsilon^{1/2} \rho u^2 \Omega^3 d^2} \times \sum_{n_1, n_f = 1}^{\infty} (1 + \tfrac{1}{2}\delta_{n_f, n_i}) \left[k_F^2 - \frac{2m^* E_0 n_i^2}{\hbar^2} \right] \times \left[k_F^2 + \frac{2m^*}{\hbar} \left[\Omega - n_f^2 \frac{E_0}{\hbar} \right] \right] \quad (14)$$

for radiation polarized in the plane of the layer. Here

$$k_F = \left[\frac{2m^* E_F}{\hbar^2} \right]^{1/2}$$

is the Fermi wave vector of the free carriers. From Eq. (14) we again see that we have an oscillatory dependence of the absorption coefficient on the thickness of the layer d. There are two types of oscillations which occur for the degenerate case, one which involves just the Fermi energy and the other which involves both the Fermi energy and the photon energy. For comparison, the absorption coefficient for a bulk degenerate semiconductor is

$$K_b = \frac{2E_d^2}{9\pi^2} \left[\frac{e^2 m^{*2} k_B T}{\hbar^8 \rho u^2 \epsilon^{1/2} c \Omega^3} \right] E_F^3 \left[1 + \frac{\hbar\Omega}{E_F} \right]^{3/2} , \quad (15)$$

where $E_F = (\hbar^2/2m)(3\pi^2 n_e)^{2/3}$. Similar but much more complicated expressions can be obtained for the free-carrier absorption coefficient when the radiation is polarized perpendicular to the plane of the layer. However, we will not present the results for this polarization in this paper both because of their very complicated nature and because for this polarization, the radiation would have to propagate in the plane of the layer. The reason for the complicated nature of the expressions for the free-carrier absorption for this polarization is the breakdown of the selection rule $n' = n$ for this polarization, which means that one has to sum over all intermediate states when one substitutes (6) and (8) into (3) since any one of the higher subbands can act as an intermediate state for the transition. For radiation polarized in the plane of the layer, on the other hand, the only intermediate states to which the transition can

occur belong to the same subband of either the initial or final state.

III. DISCUSSION

For nondegenerate carriers, the oscillatory dependence of the free-carrier absorption coefficient on the width of the layer in which the carriers are confined can be understood in terms of the subband structure which arises because of the confinement of the carriers. When the photon energy $\hbar\Omega$ is greater than the separation in energy between the various subbands, the absorption of a photon can occur with the simultaneous emission or absorption of phonons in transitions to the same or other subbands. Whenever a phonon-assisted transition to a new subband can take place, there is an inflection point in the absorption coefficient as a function of d^{-1} followed by a peak. As the width of the layer d decreases, the separation between adjacent subbands increases and when $\hbar\Omega < E_0$, the phonon-assisted transitions can only take place to states in the same subband. For layer widths such that $\hbar\Omega < E_0$, the absorption process depends just upon the rate at which the free carriers are scattered by the emission or absorption of phonons. The linear increase in the absorption coefficient with d^{-1} just reflects the linear increase of the electron-phonon scattering rate with d^{-1} predicted for the mobility of carriers confined in such a quasi-two-dimensional structure.[29–31] The situation here is reminiscent of the magnetic field dependence of the free-carrier absorption in nondegenerate semiconductors in which the carriers are confined by the quantizing magnetic fields.[25] The oscillatory behavior of the free-carrier absorption is in contrast to the steplike structure of the optical-absorption coefficient theoretically predicted for direct-intersubband transitions.[1] The predicted behavior of the free-carrier absorption seems closer to the behavior theoretically predicted taking excitonic effects into account[10] and which seems to be experimentally observed. In the latter case, sharp peaked structures are observed and these peaked structures are somewhat sharper than those we predict to occur in the free-carrier absorption. Since free-carrier absorption should occur in these quasi-two-dimensional structures except in those that are insulating, this effect should be taken into account in any comparison of the theory with experiment.

In the case where the carriers are degenerate, oscillations of the free-carrier absorption coefficient are also predicted to occur as a function of layer thickness. In this case, there are two kinds of oscillations: oscillations similar to the de Haas–Schubnikov oscillations, which occur in quantizing magnetic fields and which arise when the Fermi level passes through the bottom of a subband, and oscillations which depend upon the location of the Fermi level and the energy of the photon. Again the dependence of the free-carrier absorption coefficient on the layer width is reminiscent of what occurs in highly doped semiconductors in the presence of quantizing magnetic fields.[28]

In semiconducting superlattice or heterojunction structures, other scattering mechanisms such as ionized impurity scattering or, in polar materials, polar optical-phonon scattering can also play an important role in determining the free-carrier absorption. We would expect similar oscillatory structure in the absorption coefficient with increasing photon energy $\hbar\Omega$ and layer thickness d to occur when these other scattering mechanisms play a dominant role since the oscillatory behavior arises because of phonon- or impurity-assisted transitions between the various size-quantized subbands. However, the linear increase of the absorption coefficient with d^{-1}, which is predicted to occur when $\hbar\Omega < E_0$, will only occur when acoustic-phonon scattering is dominant since it is characteristic of the layer-thickness dependence of the acoustic-phonon scattering rate. When either ionized impurity scattering or polar optical-phonon scattering dominates the free-carrier absorption, we expect the thickness dependence of the absorption coefficient in the regime $\hbar\Omega < E_0$ to reflect the thickness dependence of the scattering rate for the particular scattering mechanism which is dominant. For example, for the case of ionized impurity scattering in a quasi-two-dimensional semiconducting structure, Fell *et al.*,[32] Price,[33] and others[34] have shown that the scattering rate decreases with decreasing layer thickness. Therefore, when ionized impurity scattering dominates the free-carrier absorption, we would expect the free-carrier absorption coefficient to decrease with decreasing layer thickness when $\hbar\Omega < E_0$. Since the absorption coefficient due to acoustic-phonon scattering increases with decreasing layer thickness, we expect acoustic-phonon scattering to dominate the scattering of the carriers in thinner layers.

In conclusion, we predict that when acoustic-phonon scattering is dominant, the free-carrier absorption coefficient should increase with decreasing layer thickness for radiation polarized in the plane of the layer. We also predict an oscillatory dependence of the absorption on the layer thickness with inflection points occurring whenever phonon-assisted transitions can occur to a higher subband. Because of the increase in the absorption with decreasing layer width, free-carrier absorption should become considerably enhanced as the width of a well or layer decreases.

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