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Infra-red free-carrier absorption due to impurity scattering in semiconducting quantum well structures

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Abstract. The theory of free-carrier absorption (FCA) is developed, in the extreme quantum limit when the carriers are assumed to populate only the lowest quantized energy level, for quasi-two and one-dimensional semiconducting quantum well structures where the carriers are scattered by ionized impurities. The radiation field is assumed to be polarized in the plane of the layer in the quasi-two-dimensional case and along the length of the wire in the quasi-one-dimensional case. Expressions for FCA are obtained for the cases where the impurities are either in the well (background impurities) or outside the well (remote impurities). Variation of FCA is numerically studied with photon frequency and well width.

Keywords. Optical properties; quantum wells; impurity scattering, infra-red free-carrier absorption.

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1. Introduction

The development of the molecular beam epitaxy (MBE) and metal organic chemical vapour deposition (MOCVD) methods has made possible the fabrication of submicron devices whose dimensions are of the order of the de Broglie wavelength of the electrons. In one such structure, electrons are confined in an active layer to form a quasi-two-dimensional (Q2D) electron gas, leading to quantum-size effects in its electrical and optical properties (Dingle 1975; Ando and Mori 1979). Of main interest in these systems has been the enhanced electron mobility. In GaAs/$Ga_{1-x}Al_x$ As prototype hetero-structures, the $Ga_{1-x}Al_x$As layer is modulation-doped while the carriers are confined in the GaAs layer because of the difference in the band gaps of GaAs and $Ga_{1-x}Al_x$As. In modulation-doped samples there are two kinds of impurities which can contribute to the scattering—impurities in the well, layer or film (background impurities (BI)) and those outside the well (remote impurities (RI)). Because of the separation of the carriers from the donor impurities from which they are ionized, the Coulomb scattering of carriers by these ionized impurities is reduced leading to high mobilities in these structures (Stormer *et al* 1981).

An alternative structure in which carrier scattering can be suppressed has been put forward by Sakaki (1980, 1981) who proposed fabricating ultrathin semiconducting wires. In such thin-wire structures the electrons behave essentially as a quasi-one-dimensional (Q1D) electron gas and scattering can occur by ionized impurities located inside the wire (BI) and outside the wire (RI) even if the thin wire is embedded in an

insulating structure. Recently, Petroff *et al* (1982) fabricated the GaAs quantum well wires (QWW) by MBE and studied some of its optical properties experimentally.

In recent years there has been growing interest in the study of free-carrier absorption (FCA) in Q2D and Q1D semiconducting quantum well structures. The FCA accounts for the absorption of photons of frequencies Ω lower than those which give rise to interband transitions, that is, $\hbar\Omega < E_g$ where E_g is the band gap of the semiconductor. The direct absorption of a photon by a free carrier is forbidden as it violates energy and momentum conservation laws. In the presence of phonons, ionized impurities or other lattice imperfections a free carrier may absorb a photon via a second order process in which the free carrier changes its momentum by scattering off the phonons or impurities. In this sense FCA is a powerful means of determining the possible scattering mechanisms and has been studied in bulk semiconductors with regard to various scattering mechanisms, one of them being the ionized impurity scattering (Fan 1956; Nag 1980). It is, therefore, also of interest to investigate FCA in Q1D and Q2D semiconducting structures, when electrons are scattered by ionized impurities.

FCA has been studied in Q2D quantum well structures when the free carriers are scattered by acoustic phonons via deformation potential coupling (Spector 1983), polar optical phonons (Adamska and Spector 1984), non-polar optical phonons (Kubakaddi and Mulimani 1985a) and ionized impurity scattering in the absence of screening (Sankeshwar *et al* 1987). The hot free-carrier intraband absorption coefficient of *n*-GaAs inversion layers has been calculated for various scattering mechanisms and compared with the experimental data deduced from far-infra-red absorptivity measurements (Vass 1986). Similarly, FCA has been investigated in QWW for the case where the carriers are scattered by acoustic phonons (Kubakaddi and Mulimani 1985b; Adamska and Spector 1986), optical phonons (Adamska and Spector 1986) and non-polar optical phonons (Kubakaddi and Mulimani 1988). In this paper, we extend the theory of FCA in Q2D and Q1D semiconducting quantum well structures to the case where electrons are scattered by screened ionized impurities. We consider the case when the radiation field is polarized in the plane of the layer in Q2D case and along the length of the wire in Q1D case. Further, we restrict ourselves to the extreme quantum limit (EQL) in which only the ground state of the system is occupied. This allows us to investigate FCA in the infra-red region as will be clear in the following section. In § 2 we present the formalism and derive expressions for FCA coefficients in Q2D and Q1D systems. Section 3 contains results and discussion.

2. Theory

The FCA coefficient α is given by (Meyer 1958)

$$\alpha = \frac{\varepsilon^{\frac{1}{2}}}{n_0 c} \sum_i (W_i^{\mathrm{abs}} - W_i^{\mathrm{em}}) f_i \tag{1}$$

where ε is the dielectric constant of the medium, n_0 the number of photons in the radiation field and f_i the carrier distribution function. The sum is over all initial states of the system. W_i^{abs} and W_i^{em} represent the transition probabilities for the absorption and emission of photons, respectively and can be calculated using the standard second

order Born golden rule approximation. These can be expressed as

$$W_i^{\text{abs,em}} = \langle W_i^{\pm}(\text{imp}) \rangle, \tag{2}$$

where $\langle\ \rangle$ denotes an appropriate average over impurity distribution with the transition probabilities $W_i^{\pm}(\text{imp})$ defined by

$$W_i^{\pm}(\text{imp}) = \frac{2\pi}{\hbar} \sum_f |\langle f|M|i\rangle|^2 \delta(E_f - E_i \mp \hbar\Omega). \tag{3}$$

The transition matrix-elements $\langle f|M|i\rangle$ are given by

$$\langle f|M|i\rangle = \sum_j \left| \frac{\langle f|H_{\text{rad}}|j\rangle\langle j|V_{\text{imp}}|i\rangle}{E_i - E_j} + \frac{\langle f|V_{\text{imp}}|j\rangle\langle j|H_{\text{rad}}|i\rangle}{E_i - E_j \pm \hbar\Omega} \right|. \tag{4}$$

Here H_{rad} is the electron-photon interaction Hamiltonian and V_{imp} is the scattering potential due to impurities. $\hbar\Omega$ is the energy of the photon and E_i and E_f denote the initial and final state energies of the electrons, respectively. The sum is over all the intermediate states j of the system. The above expressions can be evaluated in Q2D and Q1D quantum well structures using the appropriate energy eigenfunctions, eigenvalues and distribution functions.

2.1 *Q2D quantum well structures*

Adopting a single-band spherical effective mass model for the electrons confined to move in the x-y plane, the electron wavefunctions ψ_{nk} and the energy eigenvalues E_{nk} are given by

$$\psi_{nk}(x, y, z) = (2/V)^{1/2} \exp(i\mathbf{k}\cdot\mathbf{r}) \sin(n\pi z/d) \tag{5}$$

and

$$E_{nk} = \frac{\hbar^2 k^2}{2m^*} + n^2 E_0, \quad n = 1, 2, 3, \ldots \tag{6}$$

where

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

Here $\mathbf{r}$ and $\mathbf{k}$ denote the position vector and the wavevector in the x-y plane, respectively, V the volume of the material, d the thickness of the layer and m^* the effective mass of the electrons. For the energy eigenvalues given by (6) the distribution function f_{nk} for a non-degenerate electron gas can be shown to be (Kubakaddi and Mulimani 1985a)

$$f_{nk} = \left(\frac{\pi\hbar^2 n_s}{m^* k_B T \gamma}\right) \exp\left(-\frac{n^2 E_0}{k_B T}\right) \exp\left(-\frac{\hbar^2 k^2}{2m^* k_B T}\right), \tag{7}$$

where

$$\gamma = \sum_{n=1}^{\infty} \exp\left(-\frac{n^2 E_0}{k_B T}\right)$$

and n_s is the surface concentration of the electrons.

FCA is particularly important in determining the optical absorption when the carriers are confined to the lowest sub-band and the energy of the photon is insufficient to cause a transition to the next higher sub-band. In this case, the frequency and the thickness dependence of the absorption should, in particular, be sensitive to the scattering mechanism. As mentioned earlier we will, in what follows, restrict ourselves to the EQL in which the scattering of the electrons is confined to within the $n = 1$ level. For example, in GaAs layers of thickness 100 Å the energy difference between the lowest sub-band and the first excited sub-band is 168 meV which is much larger than the thermal energy $k_B T$ which is 26 meV at $T = 300$ K. Also, it may be noted that the energy of the photon, in the infra-red region, is much less than the sub-band separation.

Using the wavefunctions given by (5) we obtain for the matrix elements of the electron-photon interaction Hamiltonian

$$\langle 1, \mathbf{k}' | H_{\text{rad}} | 1, \mathbf{k} \rangle = -\frac{e\hbar}{m^*}\left(\frac{2\pi\hbar n_0}{\varepsilon \Omega V}\right)^{\frac{1}{2}} \mathbf{e}\cdot\mathbf{k}\,\delta_{k'_x,k_x}\delta_{k'_y,k_y}, \tag{8}$$

where $\mathbf{e}$ is the polarization vector of the radiation.

Impurity scattering has been studied by several workers (Hess 1979; Fell *et al* 1978; Lee *et al* 1983; Mori and Ando 1980). The impurity potential has been taken to be two-dimensional in some analysis (Fell *et al* 1978) while in others the three-dimensional nature of the potential has been taken into account (Lee *et al* 1983). In their detailed work Lee *et al* (1983) have obtained expressions for both the scattering potential and scattering rates for screened ionized impurity scattering using both the delta function model (DFM) for the probability density of the electrons and the sine function model (SFM) given by (5). Using the screened scattering potential (Lee *et al* 1983) for an impurity of charge Ze located at $z = z_0$ we obtain, in the SFM, the matrix element

$$\langle 1, \mathbf{k}' | V_{\text{imp}} | 1, \mathbf{k} \rangle = \left(-\frac{8\pi^3 Z e^2 d^2}{V\varepsilon}\right)[Q^4 + (4\pi^2 + 3S)$$

$$Q^2 + 8\pi^2 S]^{-1} I(Q, z_0) \tag{9}$$

where

$$I(Q, z_0) = \frac{Q^2}{\pi^2}\sin^2(\pi z_0/d) + 2 - \exp(-Qz_0/d)$$

$$-\exp\{-Q[1-(z_0/d)]\} \qquad \text{BI} \tag{10}$$

$$= [\exp(Q) - 1]\exp(-Qz_0/d), \quad \text{RI} \tag{11}$$

with $Q = qd$ and $q = |\mathbf{k} - \mathbf{k}'|$. $S = S_1 d = 2\pi e^2 n_s d/(k_B T\varepsilon)$, where S_1 is the screening parameter (Stern and Howard 1967) for carriers in the lowest sub-band.

In the DFM the matrix element is

$$\langle 1,\mathbf{k}'|V_{\text{imp}}|1,\mathbf{k}\rangle = \left(-\frac{2\pi Ze^2d^2}{V\varepsilon}\right)[Q+S]^{-1} \times \exp\left(-Q\left|\frac{z_0}{d}-\frac{1}{2}\right|\right) \tag{12}$$

for both BI and RI.

For scattering by BI we have for the density of ionized impurities

$$N_I(z_0) = \begin{cases} N_I, & 0 < z_0 < d \\ 0, & d < z_0. \end{cases} \tag{13}$$

Similarly, for RI we can write

$$N_I(z_0) = \begin{cases} 0, & 0 < z_0 < d \\ N_I, & d < z_0. \end{cases} \tag{14}$$

With these distributions for the impurities the average defined by (2) can be explicitly written as

$$W_i^{\text{abs,em}} = \int \mathrm{d}z_0 N_I(z_0) W_i^{\pm}(\text{imp}). \tag{15}$$

The transition probabilities $W_i^{\pm}$ can be calculated in a straightforward way using equations (3)–(6) and the matrix elements given by equations (8)–(12). Finally, using equations (1), (7) and (13)–(15), we obtain the following expressions for the FCA in a Q2D non-degenerate semiconducting structures. In the SFM

$$\alpha_{\text{Q2D}} = P\int_0^{\infty} f(X)(2x+\beta\eta^2)\exp(-x) \times [X^4+(4\pi^2+3S)X^2+8\pi^2S]^{-2}\,\mathrm{d}x, \tag{16}$$

where

$$f(X) = N_s\left[3X^4+16\pi^2\left\{X^2+\pi^2(\exp(-X)-1) \times\left(1-\frac{\exp(-X)}{X}+\frac{4X^2}{X^2+4\pi^2}\right)+3\pi^2\right\}\right] \quad \text{BI} \tag{17}$$

$$= 4\pi^4 N_I d[1-\exp(-X)]^2/X \quad \text{RI} \tag{18}$$

with

$$X = [(x+\beta\eta^2)^{\frac{1}{2}} - x^{\frac{1}{2}}]d/\beta^{\frac{1}{2}},$$

$$P = (2^4\pi^3Z^2e^6n_sdk_BT)(c^2\varepsilon^5\hbar^8)^{-\frac{1}{2}}[1-\exp(-y)]\Omega^{-3},$$

$$\beta = \hbar^2/(2m^*k_BT),$$

$$\eta^2 = 2m^*\Omega/\hbar,$$

$$y = \hbar\Omega/k_BT,$$

and N_s is the surface density of the ionized impurities. For the DFM we obtain

$$\alpha_{Q2D} = 2^{-2}P\int_0^\infty g(X)(2x+\beta\eta^2)\exp(-x)[X(X+S)^2]^{-1}\,dx, \tag{19}$$

where

$$g(X) = 2N_s[1-\exp(-X)] \quad \text{BI} \tag{20}$$

$$= N_I d\exp(-X). \quad \text{RI} \tag{21}$$

Using (16) and (19) FCA can be evaluated, numerically, as a function of Ω, d and T.

2.2 *Q1D quantum well structures*

Assuming a cylindrical geometry for a wire of radius a and length L, the eigenfunctions and eigenvalues for the electrons are (Lee and Spector 1983)

$$\psi_{nlk}(\mathbf{r}) = \frac{\exp(ikz)\exp(il\theta)J_l(k_{nl}r)}{(\pi a^2 L)^{\frac{1}{2}}J_{l+1}(k_{nl}a)}$$

$$l = 0, 1, 2, 3, \ldots, \quad n = 1, 2, 3, \ldots \tag{22}$$

and

$$E_{nlk} = (\hbar^2/2m^*)(k^2 + k_{nl}^2) \tag{23}$$

respectively, where k is the wavevector of the electron along the z direction, that is, the length of the wire, $J_l(x)$ is the Bessel function of the first kind of order l, and k_{nl} is related to the nth zero of the Bessel function of order l, that is $k_{nl} = x_{nl}/a$ where $J_l(x_{nl}) = 0$.

For the energy spectrum given by (23) the distribution function, in the non-degenerate case, can be shown to be

$$f_{nlk} = \left(\frac{2\pi^3}{m^*k_BT}\right)^{\frac{1}{2}}\left(\frac{hn_e a^2}{\delta}\right)\exp\left(-\frac{\hbar^2k_{nl}^2}{2m^*k_BT}\right)\exp\left(-\frac{\hbar^2k^2}{2m^*k_BT}\right), \tag{24}$$

where

$$\delta = \sum_{n,l}\exp\left(-\frac{\hbar^2k_{nl}^2}{2m^*k_BT}\right)$$

and n_e is the carrier concentration.

As in the case of Q2D systems we assume the electrons to be confined to their lowest quantum state ($l = 0, n = 1$). The matrix elements of the electron-photon interaction can be written as

$$\langle 1\,0\,\mathbf{k}'|H_{rad}|1\,0\,\mathbf{k}\rangle = -\frac{e\hbar}{m^*}\left(\frac{2\pi\hbar n_0}{\varepsilon\Omega V}\right)^{\frac{1}{2}}\mathbf{e}\cdot\mathbf{k}\,\delta_{\mathbf{k}',\mathbf{k}}. \tag{25}$$

Since in a very thin wire the electrons in their lowest quantum state are essentially confined along the axis of the wire, the electron probability density which enters the matrix elements for impurity interaction can be approximated by a delta function as far

as their motion transverse to the axis of the wire is concerned (Lee and Spector 1983). With this assumption the matrix elements for the unscreened Coulomb potential of an ionized impurity of charge Ze located at a distance R away from the axis of the wire, are given by

$$\langle 1\ 0\ \mathbf{k}'|V_{\text{imp}}|1\ 0\ \mathbf{k}\rangle = [-Ze^2/(2\pi\varepsilon L)]K_0(qR), \tag{26}$$

where $K_n(x)$ is the modified Bessel function of the second kind of order n, and $q = |\mathbf{k} - \mathbf{k}'| = 2k$.

A proper treatment of screening involves evaluation of complicated integrals (Lee and Spector 1985). To a first approximation, in order to understand the role of impurities, earlier workers considered the scattering of electrons by either unscreened ionized impurities (Lee and Spector 1983) or assumed the Coulomb interaction to be screened by the static dielectric constant of the material (Brown and Spector 1986). However, in the simplest approximation, we can incorporate (Lee and Vassell 1984) the effect of screening by replacing ε in (26) by $\varepsilon\varepsilon_{\text{TF}}$ where ε_{TF} is the dielectric function for a 1D system obtained using Thomas-Fermi approximation

$$\varepsilon_{\text{TF}} = 1 + [(4\pi n_l e^2)/(k_B T\varepsilon)]$$

with n_l being the electron density per unit length.

For scattering from BI, we assume that the density of ionized impurities is uniform inside the wire and is a function of only the distance R and vanishes outside

$$N_I(R) = \begin{cases} N_I, & R < a \\ 0, & R > a. \end{cases} \tag{27}$$

In the case of scattering by RI, the impurity density vanishes inside the wire and is uniformly distributed outside the wire

$$N_I(R) = \begin{cases} 0, & R < a \\ N_I, & R > a. \end{cases} \tag{28}$$

For these distributions the impurity averages of transition probabilities can be expressed as

$$W_i^{\text{abs,em}} = \int \mathrm{d}^3 R N_I(R) W_i^{\pm}. \tag{29}$$

Now the FCA coefficient can be evaluated as in the case of Q2D systems. We obtain

$$\alpha_{\text{Q1D}} = (2\pi)^{-\frac{1}{2}} P_1 \int_0^\infty f(\mu)(x^2 + 4a^2\eta^2)^{-\frac{1}{4}} \exp(-\beta x^2/(4a^2))\mathrm{d}x, \tag{30}$$

where

$$f(\mu) = 1 - \mu \quad \text{BI}, \tag{31}$$

$$= \mu \quad \text{RI}, \tag{32}$$

with

$$\mu = x^2\{K_1^2(x) - K_0^2(x)\}$$

and

$$P_1 = (Z^2e^6N_In_e)(\hbar^2c^2\varepsilon^5m^{*3}k_BT)^{-\frac{1}{2}}\Omega^{-3}[1 - \exp(-y)].$$

Expression (30) can be considerably simplified in the limit $ka << 1$. This condition is just that the de Broglie wavelength of the carriers is greater than the radius of the wire and equivalent to the EQL (Lee and Spector 1983). In this limit we obtain the following analytical expression for FCA:

$$\alpha_{Q1D} = (2^3\hbar^7\varepsilon^5\Omega^7c^2m^*)^{-\frac{1}{2}}(Z^2e^6N_In_ea^2k_BT)[1 - \exp(-y)]I_1, \tag{33}$$

where

$$I_1 = \{C + \ln(\beta/a^2)\}\{C + \ln(\beta/a^2) - 4\} + \pi^2/2 \qquad \text{BI} \tag{34}$$

$$= 2(\beta/a^2) - [\{C + \ln(\beta/a^2)\}\{C + \ln(\beta/a^2) - 4\} + \pi^2/2] \qquad \text{RI} \tag{35}$$

with $C = 0{\cdot}577215$, the Euler's constant.

3. Results and discussion

We have performed calculations of FCA coefficient in Q2D and Q1D systems at 77 K for parameters characteristic of GaAs in bulk. The values for the various quantities used are:

$m^* = 0{\cdot}07\,m_e$, $\varepsilon = 11{\cdot}56$;

Q2D: $N_I = 10^{17}\,\text{cm}^{-3}$, $N_s = 10^{11}\,\text{cm}^{-2}$ and $n_s = 1 \times 10^{10}\,\text{cm}^{-2}$, $5 \times 10^{10}\,\text{cm}^{-2}$.

Q1D: $n_e = N_I = 10^{16}\,\text{cm}^{-3}$.

Figure 1 shows the variation of α_{Q2D}, calculated using SFM (equation (16)), with photon frequency Ω. From the figure it can be seen that α_{Q2D} decreases with increase of Ω. For the values of layer thicknesses used, the contribution to FCA from background impurity scattering (BIS) is seen to be greater than that from remote impurity scattering (RIS). Curves 1, 2, 3 and 4, in each case, show the variation of absorption with surface carrier density n_s in the layer and with layer thickness d. In both cases, for a particular frequency, FCA increases with decrease of d. However, in both cases, for a particular frequency, FCA increases with increase of n_s.

In figure 2 we have plotted α_{Q2D}, for the DFM (equation (19)), as a function of Ω. The behaviour of FCA is similar to that for SFM.

In figure 3 we have plotted α_{Q1D} as a function of Ω for both the BIS and RIS cases. Curves 1 and 2, in each set, correspond to the values calculated using the exact equation (30). The broken curves have been plotted for $a = 50$ Å using (33) obtained under the approximation $ka \ll 1$. From the figure it is seen that FCA decreases with Ω. For BI it increases with a, the radius of the wire. However, in the case of RI it decreases with the

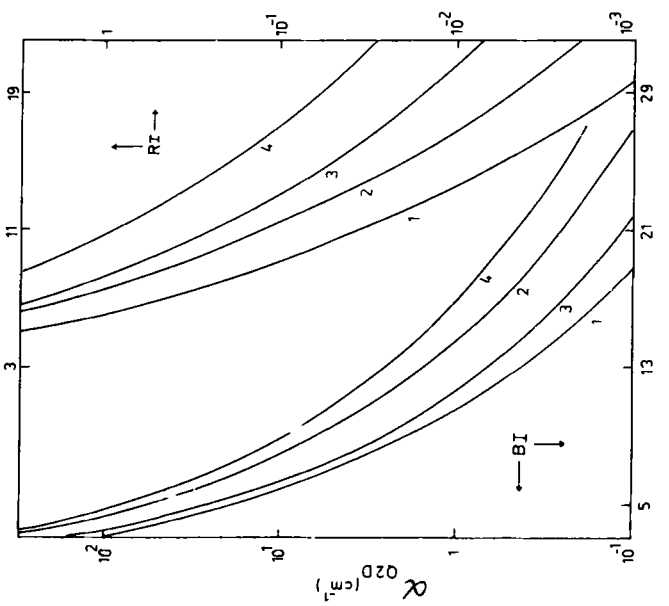

Figure 2. Free-carrier absorption for background and remote impurity scattering is shown in Q2D system in delta function model as a function of photon frequency at $T = 77$ K. Curve 1: $n_s = 1 \times 10^{10}$ cm^{-2}, $d = 100$ Å; curve 2: $n_s = 5 \times 10^{10}$ cm^{-2}, $d = 100$ Å; curve 3: $n_s = 1 \times 10^{10}$ cm^{-2}, $d = 50$ Å; curve 4: $n_s = 5 \times 10^{10}$ cm^{-2}, $d = 50$ Å.

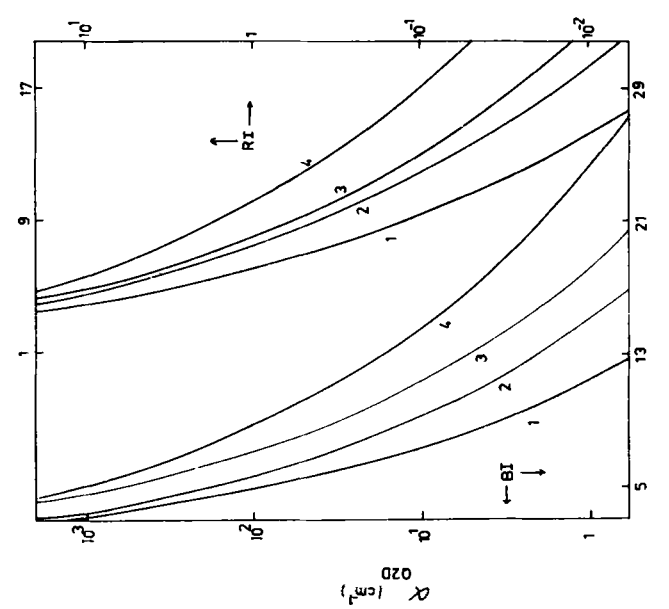

Figure 1. Free-carrier absorption for background and remote impurity scattering is shown in Q2D system in sine function model as a function of photon frequency at $T = 77$ K. Curve 1: $n_s = 1 \times 10^{10}$ cm^{-2}, $d = 100$ Å; curve 2: $n_s = 5 \times 10^{10}$ cm^{-2}, $d = 100$ Å; curve 3: $n_s = 1 \times 10^{10}$ cm^{-2}, $d = 50$ Å; curve 4: $n_s = 5 \times 10^{10}$ cm^{-2}, $d = 50$ Å.

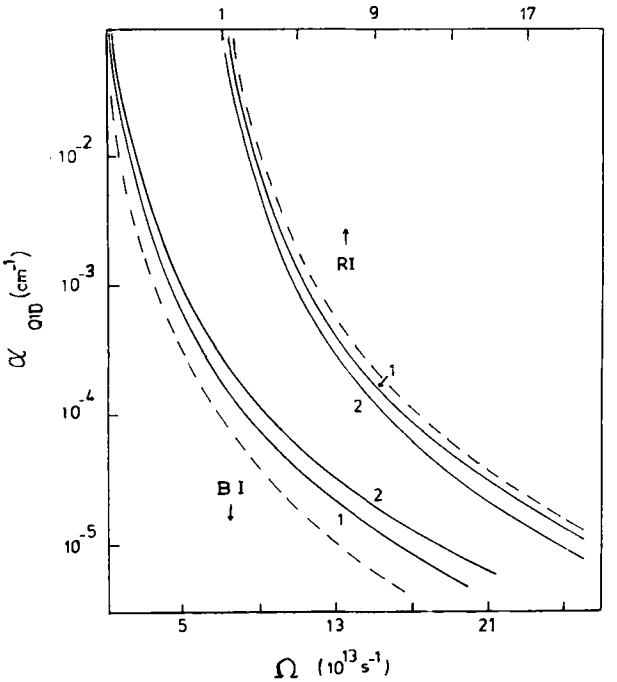

Figure 3. Free-carrier absorption for background and remote impurity scattering is shown in Q1D system as a function of photon frequency at $T = 77$ K and $a = 25$ Å (curve 1) and 50 Å (curve 2). The broken curves (equation (33)) refer to $a = 50$ Å.

increase of a. The effect of incorporation of screening, as discussed earlier, via replacement of ε by $\varepsilon\varepsilon_{TF}$ will be to reduce the FCA. The behaviour of FCA with photon frequency is not expected to alter.

The values of α_{Q2D} and α_{Q1D} due to impurity scattering can be compared with those due to acoustic phonon scattering. For $T = 77$ K, $\Omega = 9 \times 10^{13}\,s^{-1}$ and deformation potential constant $E_d = 7$ eV we obtain $\alpha_{Q2D} = 9{\cdot}24\,cm^{-1}$ for $d = 100$ Å (Spector 1983) and $\alpha_{Q1D} = 3{\cdot}29\,cm^{-1}$ for $a = 50$ Å (Kubakaddi and Mulimani 1985b). Also, we can compare the results with those due to impurity scattering in bulk semiconductor. For example, for $\Omega = 9 \times 10^{13}\,s^{-1}$, $T = 77$ K and the values of parameters used in the calculations the value of α in bulk semiconductor (Fan 1956) is $5{\cdot}42 \times 10^{-2}\,cm^{-1}$.

In conclusion, we have studied the behaviour of FCA coefficient due to scattering by background and remote impurities in Q2D and Q1D semiconducting quantum well structures as a function of photon frequency and well width. It would be interesting to see the experimental results for FCA in these structures to test the predictions of the present work.

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