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1990 J. Phys.: Condens. Matter 2 5613

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# Resonances of intraband absorption of infrared radiation in semiconductors

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Received 24 July 1989, in final form 5 February 1990

**Abstract.** The effect of the internal structure of an impurity centre on the bremsstrahlung absorption processes of infrared radiation by free carriers in semiconductors has been analysed. It is shown that the presence of a bound current carrier in the impurity level significantly influences the frequency dependence of the intraband absorption coefficient.

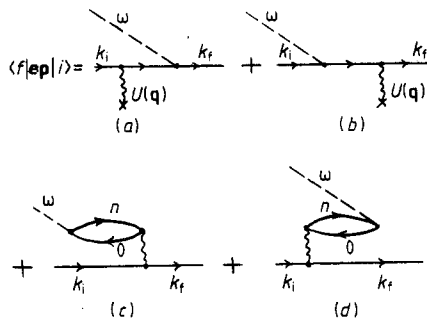
## 1. Introduction

When considering intraband absorption connected with the scattering of free carriers by impurity centres, one usually starts from the similarity existing between this process and bremsstrahlung absorption by a fast electron in the field of an isolated atom. If the majority of impurities in a crystal are in an ionised state, it is assumed that the intraband absorption occurs because of scattering of carriers by a Coulomb field of centres (Fan *et al* 1956, Meyer 1958, Wolfe 1954). The coefficient  $\eta(\omega)$  of intraband absorption in this case is a monotonic function of photon frequency  $\omega$ . If the majority of impurity levels are filled, bremsstrahlung absorption occurs during free-carrier scattering by non-ionised impurity centres. In this case the amplitude of the bremsstrahlung absorption is represented by the Feynman graphs in figure 1. Figures 1(a) and 1(b) correspond to direct absorption of quanta by a free carrier in the field of a non-ionised centre. Figures 1(c) and 1(d) represent a two-stage process. In the first stage of this process, excitation of the bound carrier occurs; in the second stage this carrier returns to the ground state of the centre. At the same time the excitation energy transfers to a free carrier. Coulomb interaction between free and bound carriers in these diagrams is included in the lowest relevant order of perturbation theory. Evidently, in the case of the ionised centre diagrams in figures 1(c) and 1(d) it is absent. On increase in the frequency  $\omega$ , figures 1(c) and 1(d) play the leading part of the function  $\eta(\omega)$ , as will be shown below, becomes non-monotonic. Resonances connected with discrete excitations of an impurity carrier appear in this function.

The present paper is dedicated to the research of resonances in the intraband absorption coefficient.

## 2. Cross section of the bremsstrahlung absorption

When calculating the cross section of bremsstrahlung absorption by the impurity centre, we shall assume that the ground-state level of a centre lies fairly asymmetrically



**Figure 1.** Diagrammatic representation of the bremsstrahlung amplitude. The full lines describe the accelerating carrier moving in the field of the centre and the broken lines denote an absorption quantum  $\omega$ . The wavy lines in (a) and (b) denote the static interaction  $U(q)$  between the free carrier and impurity centre. The wavy lines in (c) and (d) describe the Coulomb interaction between free and bound charges. The symbols 0 and  $n$  correspond to the ground and excited states of the impurity centre.

with respect to the middle of the gap. This condition enables us to assume that the ground-state wavefunction is formed from Bloch functions of the nearest band, whose dispersion relation is quadratic. The description of such centres (e.g. elemental impurities of groups III and V in germanium and silicon) is based on their presentation as a model atom in a homogeneous medium with a certain permittivity. It is clear that such a description is reasonable when the size of the orbit of the centre ground state sufficiently exceeds the lattice constant, i.e. in those cases when the effective mass  $m^*$  of the carriers is small and the permittivity  $\epsilon_0$  of the material is large. Interaction of the carrier with the impurity 'nucleus' in the model atom is approximated by a single-particle potential  $V(r_1)$  which is a short-range potential for a deep impurity (Lucovsky 1965), a Coulomb potential for shallow levels (Luttinger and Kohn 1955) and a Coulomb potential with a short-range nature for centres with the ground level location at an intermediate depth (Baltenkov and Grinberg 1976). Within the framework of such a model, the free-carrier scattering by the impurity centre is given by the Schrödinger equation

$$[-\frac{1}{2}(\Delta_1 + \Delta_2) + V(r_1) + V(r_2) + 1/|r_1 - r_2| - E_{i,f}] \psi_{i,f}^{\pm} = 0. \quad (1)$$

Here  $E_{i,f}$  are the energies measured from the band edge,  $r_1$  and  $r_2$  are the radii vectors of carriers on the impurity level and in the band, respectively and  $\psi_i^+(r_1, r_2)$  and  $\psi_f^-(r_1, r_2)$  are wavefunctions of the system (impurity and free carrier) before and after quantum absorption, respectively. In equation (1) and below, 'atomic' units are used ( $\hbar = m^* = e^2/\epsilon_0 = 1$ ), where  $a_0^* = \hbar\epsilon_0/m^*e^2$  is the effective Bohr radius in the solid;  $m^*e^4/\hbar^2\epsilon_0^2 = 2 \text{ Ryd}^*$  is the effective atomic unit of energy.

Solutions of this equation describing the process of bremsstrahlung absorption at  $r_2 \rightarrow \infty$  should have the shape of a spherical wave diverging ( $\psi_i^+$ ) and converging ( $\psi_f^-$ ) along this coordinate. To find the solutions of (1) with these boundary conditions we write the wavefunctions as an expansion by the eigenfunctions  $\varphi_n(r_1)$  of the impurity centre defined by the following equation:

$$(-\frac{1}{2}\Delta_1 + V(r_1) - E_n)\varphi_n(r_1) = 0. \quad (2)$$

Substituting this expansion into equation (1) and using the orthonormality of the functions  $\varphi_n(r_1)$ , we write the wavefunctions of the system before and after photon absorption as follows:

$$\begin{aligned} \psi_i^+ &= \exp(ik_i \cdot r_2) \varphi_0(r_1) + \sum_n \varphi_n(r_1) \int G_{k_n}^+(r_2, r_2') U_{nE_i}(r_2') dr_2' \\ \psi_f^- &= \exp(ik_f \cdot r_2) \varphi_0(r_1) + \sum_m \varphi_m(r_1) \int G_{k_m}^-(r_2, r_2') U_{mE_f}(r_2') dr_2'. \end{aligned} \quad (3)$$

Expansion (3) includes as usual the relevant integrals of the impurity continuum spectrum. It is assumed that the bound carrier after the photon absorption remains in the ground state  $\varphi_0(\mathbf{r}_1)$  with the ionisation potential  $I_0$ . In equation (3),  $k_n^2/2 = E_i - E_n$ ,  $k_m^2/2 = E_f - E_m$ ,  $G_{\bar{k}}^{\pm}(\mathbf{r}, \mathbf{r}')$  are Green functions of free motion and  $U_{nE}(\mathbf{r}_2)$  is defined by the integral

$$U_{nE_{i,f}}(\mathbf{r}_2) = \int \varphi_n^*(\mathbf{r}_1) \left( \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} + V(\mathbf{r}_2) \right) \psi_{i,f}^{\pm}(\mathbf{r}_1, \mathbf{r}_2) d\mathbf{r}_1. \quad (4)$$

The differential cross section of the bremsstrahlung quantum absorption with polarisation  $\mathbf{e}$  related to the space angle  $d\Omega_{k_f}$ , in which the momentum of the carrier in the final state appears, is determined by

$$d\sigma_e/d\Omega_{k_f} = (k_f/2\pi c\bar{n}\omega) |\langle f|\mathbf{e} \cdot \boldsymbol{\rho}|i\rangle|^2. \quad (5)$$

Here  $\bar{n}$  is the refractive index in a crystal at the frequency  $\omega$ . The dipole matrix element is

$$\langle f|\mathbf{e} \cdot \boldsymbol{\rho}|i\rangle = -i \iint \psi_f^{-*}(\mathbf{r}_1, \mathbf{r}_2) \mathbf{e} (\nabla_1 + \nabla_2) \psi_i^+(\mathbf{r}_1, \mathbf{r}_2) d\mathbf{r}_1 d\mathbf{r}_2. \quad (6)$$

Let us consider radiation absorption by free carriers when their kinetic energy is large in comparison with  $I_0$ . In this case we can confine ourselves in (3) to terms of first order on the interaction of the free charge with the impurity centre. Calculating the matrix element (6) in the first Born approximation, we get for  $\omega \ll k_f^2/2 \approx k_i^2/2$  the following formula for the dipole moment:

$$\langle f|\mathbf{e} \cdot \boldsymbol{\rho}|i\rangle = -(\mathbf{e} \cdot \mathbf{q}/\omega) [U(\mathbf{q}) + 4\pi(\omega^2/q^2)\alpha(\omega, \mathbf{q})]. \quad (7)$$

Here  $\mathbf{q} = \mathbf{k}_i - \mathbf{k}_f$  is the momentum transferred during collision,

$$U(\mathbf{q}) = \iint \exp(i\mathbf{q} \cdot \mathbf{r}_2) |\varphi_0(\mathbf{r}_1)|^2 \left( \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} + V(\mathbf{r}_2) \right) d\mathbf{r}_1 d\mathbf{r}_2 \quad (8)$$

is the Fourier image of the static potential of field created by the filled impurity centre;

$$\alpha(\omega, \mathbf{q}) = \frac{2}{i(\mathbf{e} \cdot \mathbf{q})} \sum_n \frac{(I_0 + E_n)(\mathbf{e} \cdot \mathbf{r}_1)_{0n} [\exp(i\mathbf{q} \cdot \mathbf{r}_1)]_{n0}}{(I_0 + E_n)^2 - \omega^2} \quad (9)$$

is the generalised polarisability of the impurity atom in the ground state (Amusia *et al* 1977, 1985) converted into a common dynamical polarisability of the centre  $\alpha_d(\omega)$  at  $q \rightarrow 0$ . The matrix elements  $(\mathbf{e} \cdot \mathbf{r}_1)_{0n}$  and  $[\exp(i\mathbf{q} \cdot \mathbf{r}_1)]_{n0}$  appearing in (9) are calculated by means of the complete set of eigenfunctions of equation (2).

According to equation (7), the amplitude of the bremsstrahlung absorption on the filled impurity centre comprises the amplitude of quantum absorption by the free carrier in the static field of the impurity  $\sim U(\mathbf{q})$  and the amplitude of the coherent process  $\sim \alpha(\omega, \mathbf{q})$  passing through the virtual excitation of the bound carrier.

The cross section of the process in the case of non-polarised radiation according to (5) is expressed as

$$\sigma_{k_i}(\omega) = \frac{1}{3c\bar{n}\omega^3 k_i} \int_{k_f - k_i}^{k_f + k_i} |U(\mathbf{q}) + 4\pi \frac{\omega^2}{q^2} \alpha(\omega, \mathbf{q})|^2 q^3 dq. \quad (10)$$

At small  $q$  the main contribution in the integral is given by the second term; near the

upper limit,  $U(\mathbf{q})$  becomes significant in (10) because at large transferred momentum  $\alpha(\omega, \mathbf{q})$  is close to zero owing to the presence of the rapidly oscillating factor  $[\exp(i\mathbf{q} \cdot \mathbf{r}_1)]_{n0}$  in (9). Integrating the squares of the first and the second terms in (10) in those ranges of  $q$  where each of them is large we obtain the following approximate expression for the cross section:

$$\sigma_{k_i}(\omega) = \frac{16\pi^2}{3} \frac{1}{c\bar{n}\omega^3 k_i} \left[ \frac{1}{16\pi^2} \int_{1/\rho_0}^{2k_i} |U(\mathbf{q})|^2 q^3 dq + \omega^4 |\alpha_d(\omega)|^2 \ln\left(\frac{k_i}{\omega\rho_0}\right) \right]. \quad (11)$$

Here  $\rho_0$  is the effective radius of the filled centre. The logarithmic approximation (Zon 1977) used to obtain this formula is valid when the logarithm argument in (11) is much greater than unity, i.e. ( $k_i/\omega\rho_0 \gg 1$ , and  $k_i\rho_0 \gg 1$ ).

The first term in (11) is the cross section of the bremsstrahlung absorption in the static field of the impurity and it monotonically decreases with increasing photon energy. The second term is characterised by a more complicated frequency dependence: in the long-wave range ( $\omega \rightarrow 0$ ) it is small and at  $\omega \rightarrow \omega_s$  ( $\omega_s$  is the frequency of the dipole excitation of the bound current carrier in the impurity) it has a resonance nature because of the presence of the poles in the dynamic polarisability  $\alpha_d(\omega)$  caused by real excitations of the impurity carrier.

### 3. The intraband absorption coefficient

The intraband absorption coefficient connected with the scattering of free carriers by impurity centres is defined as

$$\eta(\omega) = NN_a [1 - \exp(-\omega/T)] \int f(k_i) \sigma_{k_i}(\omega) dk_i \quad (12)$$

where  $N$  and  $N_a$  are the concentrations of free carriers and impurity centres, respectively,  $T$  is the crystal temperature in energy units and  $f(k_i)$  is the distribution function for the carriers in band normalised by the condition  $\int f(k_i) dk_i = 1$ .

For shallow impurities described by a hydrogen-like model (Luttinger and Kohn 1955) over a wide range of free carrier rates,  $|U(\mathbf{q})| \approx 20\pi/k_i$  (Erginsoy 1950) and  $\rho_0 \approx a_0^*$ . In the case of the classical distribution of  $f(k_i)$  integration of (12) results in the following expression for  $\eta_s(\omega)$ :

$$\eta_s(\omega) = \eta_0(\omega) \left\{ (15/\pi)(T/\text{Ryd}^*)^{3/2} + \frac{1}{4} (\hbar\omega/\text{Ryd}^*)^4 |\alpha_d(\omega)/a_0^{*3}|^2 [\ln(2\sqrt{T \text{Ryd}^*/\hbar\omega}) - \gamma/2] \right\} \quad (13)$$

where  $\gamma$  is Euler's constant and  $\eta_0(\omega)$  in common units is

$$\eta_0(\omega) = (4\sqrt{2}\pi^{3/2}/3.137\bar{n}) NN_a (\hbar e^4/\epsilon_0^2 m^{*3/2} \omega^2 T^{3/2}). \quad (14)$$

The dynamic polarisability  $\alpha_d(\omega)$  of a hydrogen-like atom in (13) is defined by the formula

$$\alpha_d(\omega) = 4a_0^{*3} (\text{Ryd}^*/I_0)^2 (\text{Ryd}^*/\hbar\omega)^2 (M_+ + M_- - 1) \quad (15)$$

(Zon *et al* 1968), where

$$M_{\pm} = [2(\beta k_{\pm})^2/(2 - \beta k_{\pm})(1 + \beta k_{\pm})^2] {}_2F_1\{1, -1 - \beta k_{\pm}; 3 - \beta k_{\pm}; [(1 - \beta k_{\pm})/(1 + \beta k_{\pm})]^2\}. \quad (16)$$

Here,  $\beta = (\text{Ryd}^*/I_0)^{1/2}$ ,  $k_{\pm} = (1 \pm \lambda)^{-1/2}$  and  $\lambda = \hbar\omega/I_0$ .  ${}_2F_1(a, b; c; z)$  is a hypergeometrical function (Bateman and Erdelyi 1953). The polarisability of the shallow centre (15) at  $\beta k_{\pm} = 2, 3, 4, \dots$  has a set of poles. These poles correspond to the resonances of excited p states of the impurity.

In the case of the deep impurities described by the Lucovsky model (Lucovsky 1965) the static potential of the filled centre can be approximated by the screened Coulomb potential  $U(q) = -4\pi/(q^2 + l_D^{-2})$ , where  $l_D = (T/4\pi N)^{1/2}$  is a Debye screening radius. The dynamic polarisability of the deep impurity level is determined by the expression (Baltenkov and Gilerson 1980)

$$\alpha_d(\omega) = 4a_0^*{}^3 (\text{Ryd}^*/\hbar\omega)^2 [-1 - 8/3\lambda^2 + (4/3\lambda^2)(k_+^{-3} + k_-^{-3})]. \quad (17)$$

Substitution of (17) into (11) and integration over  $q$  (in this case  $\rho_0 \sim l_D$ ) gives the following expression for the absorption coefficient:

$$\eta_d(\omega) = \eta_0(\omega) \{2[\ln(T/E_D) - \gamma] + \frac{1}{4}(\hbar\omega/\text{Ryd}^*)^4 |\alpha_d(\omega)/a_0^*{}^3|^2 \times [\ln(2\sqrt{TE_D}/\hbar\omega) - \gamma/2]\} \quad (18)$$

where  $E_D = \hbar^2/2m^*l_D^2$ . The deep centre in the model (Lucovsky 1965) does not form excited states and thus  $\alpha_d(\omega)$  (17) as a function of  $\omega$  in contrast with shallow centres has no resonances.

The intraband absorption at impurity centres with intermediate depth of the ground level (Baltenkov and Grinberg 1976) is expressed by equation (18) where  $E_D$  is substituted by  $I_0$  and  $\alpha_d(\omega)$  is given in the paper by Baltenkov and Gilerson (1980):

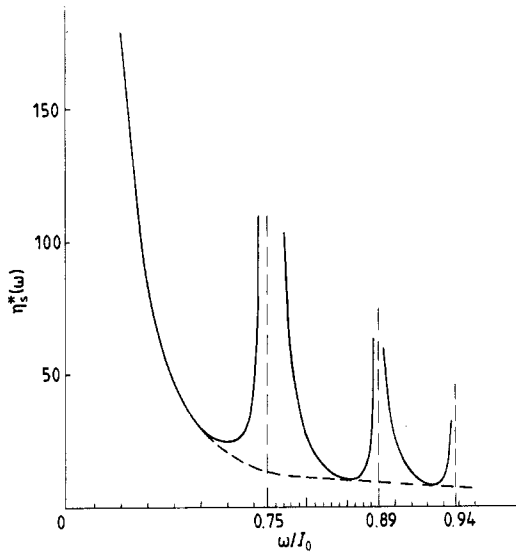
$$\alpha_d(\omega) = a_0^*{}^3 (\text{Ryd}^*/I_0)^2 [{}_2F_1(1, -1 - \beta k_+; 3 - \beta k_+; z_+)/ (2 - \beta k_+) (1 + \sqrt{1 + \lambda})^2 + {}_2F_1(1, -1 - \beta k_-; 3 - \beta k_-; z_-) / (2 - \beta k_-) (1 + \sqrt{1 - \lambda})^2] \quad (19)$$

where  $z_{\pm} = (1 - k_{\pm})^2 / (1 + k_{\pm})^2$  and  $\beta = z(\text{Ryd}^*/I_0)^{1/2}$ .

The frequency dependence of the absorption coefficient  $\eta_i(\omega)$  in this case is significantly different for attracting ( $z > 0$ ) and repulsing ( $z < 0$ ) centres. In the first case,  $\eta_i(\omega)$  according to (19) contains a Rydberg set of poles caused by the presence of excited bound states in attracting centres. In the second case there are no discrete excitations and  $\eta_i(\omega)$  has no resonances.

Figure 2 presents a  $\eta_s(\omega)$  frequency dependence calculated from equation (13). It is seen from the figure that the bound carrier significantly changes the cross section behaviour at  $\omega \leq I_0$ . A similar behaviour is typical for the absorption coefficient for attracting impurity centres at the intermediate depth. Calculations showed that the resonance peaks in the absorption coefficient become narrower on increase in crystal temperature, but the frequency dependence does not change significantly. In the case of deep and repulsing centres which have no excited states, polarisation absorption occurs only at quantum energies significantly exceeding the impurity ionisation potential when the intraband absorption is masked by the centre photoionisation processes. At lower frequencies the contribution to  $\eta(\omega)$  of the absorption caused by the bound carriers appears to be negligible and the process is assumed to occur in a static field of the centre.

It is known that the intraband infrared radiation absorption in semiconductors is accompanied by the drag effect of free carriers. The value of the drag current is determined by the coefficient of intraband absorption (Grinberg 1986). Thus, in those cases when the drag current is formed on account of bremsstrahlung absorption on impurities



**Figure 2.** Intraband absorption coefficient  $\eta_s^*(\omega) = \eta_s(\omega)\bar{n}/NN_0a_0^5$  as a function of frequency  $\omega$  at  $I_0 = \text{Ryd}^*$  and  $T = 2 \text{ Ryd}^*$ . The full curves are the calculation result taking impurity polarisation into account and the broken curve is the static approximation. A uniform scale between poles understandable from the figure was chosen.

at radiation frequencies  $\omega \rightarrow \omega_s$ , there should be resonances specified by the structure of the impurity centres.

Thus the frequency dependence of the coefficient of intraband infrared radiation absorption in semiconductors is determined to a great extent by the nature of the interaction of the bound carriers in the impurity. Therefore, investigation of the absorption resonances could be a method for obtaining information about the impurity centre structure.

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