

Far infrared absorption by donor pairs in strongly compensated semiconductors

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1990 J. Phys.: Condens. Matter 2 9435

(<http://iopscience.iop.org/0953-8984/2/47/017>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.151

The article was downloaded on 11/05/2010 at 07:00

Please note that [terms and conditions apply](#).

Far infrared absorption by donor pairs in strongly compensated semiconductors

T Szwacka† and J Blinowski

Institute of Theoretical Physics, Warsaw University, ul. Hoza 69, 00-681 Warsaw, Poland

Received 5 February 1990, in final form 18 May 1990

Abstract. The effect of electric field and potential energy fluctuations on the absorption spectrum of shallow donors in strongly compensated semiconductors has been investigated. The ionized donor pairs D_2^- with various interdonor separations and various degrees of polarity are shown to give rise to the broad absorption maximum at photon energies above that of the $1s-2p$ transition in an isolated donor atom. The height and shape of this maximum, depending on donor concentration, compensation and effectiveness of screening, carry information about the magnitude of potential energy fluctuations in strongly compensated semiconductors.

1. Introduction

The strongly compensated semiconductors represent an interesting class of materials for both technological and fundamental research reasons. The technological importance became evident with the development of GaAs-based electronics, where the semi-insulating, strongly compensated crystals serve as a basic material for the device technology. In fundamental research the strongly compensated semiconductor represents a model case of a disordered system with the large spatial fluctuations of the electronic potential energy.

Despite considerable experimental and theoretical efforts [1] our understanding of the physical properties of strongly compensated materials is far from being complete. In particular, little is known about optical absorption spectra due to shallow impurities in these materials. The far infrared magneto absorption spectra obtained by Paget and Klein for compensated n-type GaAs in 1986 [2] exhibit an absorption peak at the energy of the $1s-2p$ transition of isolated shallow donors superimposed on a featureless absorption band. The band was tentatively attributed by these authors to optical transitions involving 'deeper donors', i.e. unidentified centres with various binding energies higher than for isolated shallow donors. The absorption spectra studied by Paget and Klein refer to a quite complex experimental situation involving the application of red light illumination and very high magnetic fields to the samples with unspecified donor and acceptor concentrations. Even though it was hard to draw quantitative conclusions it was verified that the broad absorption band resulted from the presence of a high

† Permanent address: Departamento de Física, Facultad de Ciencias, Universidad de Los Andes, Mérida, Venezuela.

concentration of charged positive and negative impurity centres typical for semi-insulating compensated materials. The spectra observed by Paget and Klein represent a challenge, in particular when compared with the far infrared absorption spectra recorded by Arendarchuk and co-workers [3] for weakly doped, strongly compensated n-type InSb.

These InSb spectra exhibit several absorption peaks, interpreted by the authors as being due to different allowed transitions within ionized donor pairs D_2^+ with the largest interdonor separations having the ground state energy equal to the Fermi energy. The interpretation proposed by Arendarchuk and co-workers [3] is based on the model of isolated donor pairs and neglects completely the surrounding charged impurities. Its relative success in explaining the recorded spectra is somewhat surprising since for a random distribution of charged impurities the field and potential fluctuations in strongly compensated materials seem to be quite important and not limited to the nearest-neighbour effects.

To the best of our knowledge, there exists no quantitative theory of the effect of electric field and potential energy fluctuations on the far infrared absorption spectra of strongly compensated semiconductors. This paper aims to construct such a theory. We are interested in the region of photon energies above that of the 1s–2p transition for isolated impurities. We focus our attention on the effects due to impurity pairs; this imposes upper limits on impurity concentrations and compensations. Obviously we are interested in compensated materials with the Fermi level coinciding with some shallow impurity states. Our definition of strongly compensated materials is therefore somewhat different to the standard one. We consider the material to be strongly compensated when the number of shallow majority centres is slightly larger than the total number of minority centres.

Rigorous analysis of the variations of fields and potentials in strongly compensated semiconductors is so complicated [1] that for practical purposes simplified phenomenological descriptions have been proposed [1, 4]. They amount to replacing the Coulomb potentials of impurity ions by Yukawa potentials with the screening length λ determined by a numerical self-consistent calculation [4, 5]. In the present work we use order of magnitude estimates of λ for a completely random distribution of impurities and we introduce a numerical uncertainty prefactor. To visualize the effect of the field and potential fluctuations we compare the optical spectra calculated for the n-type strongly compensated GaAs with different values of the uncertainty prefactor.

Our results shed light on the origin of ‘deeper donors’ observed by Paget and Klein [2]. We believe that ‘deeper donors’ are just singly ionized donor pairs, D_2^+ . In the presence of field and potential fluctuations donor pairs with different interdonor separations, different degrees of polarity and different Stark shifts are simultaneously populated so that absorption is possible in a broad range of photon energies and no fine structure observed by Arendarchuk and co-workers [3] is predicted. Our results seem to indicate that the fluctuations of fields and potentials in the n-type InSb samples studied by those authors were completely suppressed—either by a strong correlation in the positions of donors and acceptors in the crystal lattice (e.g. due to ionic diffusion) or by some mechanism of screening much more effective than theoretically predicted. Our results indicate that far infrared spectra may yield information on the magnitude of electrostatic fields and potentials in strongly compensated semiconductors.

The paper is organized as follows. In section 2 we outline our model and we discuss the distribution of electric fields and potentials in a compensated material. In section 3

we discuss the energy spectrum of an ionized donor pair in an external electric field and we calculate the Fermi energy. In section 4 we derive the formula for the absorption coefficient due to ionized donor pairs D_2^+ . Section 5 contains the discussion of our numerical results and some conclusions.

2. Pair model

We consider a weakly (or moderately) doped, strongly compensated semiconductor with N_D shallow, hydrogen-like donors and $N_A < N_D$ acceptors per unit volume. Qualitatively the case of a p-type material is quite similar but the complicated acceptor wavefunctions make the quantitative treatment more difficult. At low temperatures all acceptors are ionized and the number of electrons sitting on donors, $N_D - N_A$, is much smaller than the number of donor sites, N_D . Note that the simultaneous presence in the crystal of the arbitrary concentration of deep donor centres, e.g. EL2 centres in GaAs, is irrelevant since all such donors in these circumstances are neutral. In the following we will therefore ignore deep donors. With $N_D - N_A \ll N_D$ at low temperatures the occupied electronic states are localized: electrons are bound to donor ions or their clusters. The notions of a single donor and a cluster (pair, triple, etc) in a random distribution of impurities are defined somewhat arbitrarily. The definitions involve the hopping integral W_{AB} known from the elementary LCAO calculation of an ionized hydrogen molecule H_2^+ :

$$W_{AB} = \langle A | V_A | B \rangle - \langle A | B \rangle \langle A | V_B | A \rangle$$

where $|A\rangle$ and $|B\rangle$ are the ground states of an electron bound to ions A and B, V_A and V_B are the potential energies of an electron in the Coulomb field of the ions A and B, respectively. When the two donor ions, A and B, are put in an external field varying slowly in space the energy spectrum of an electron bound to these donors, as well as the electronic wavefunctions, depend crucially on the ratio $|W_{AB}/\Delta|$, where Δ is the difference of the external potentials V at the positions of the two donors. In the limiting case of the homopolar pair, with $|W_{AB}/\Delta| \gg 1$, the electron is equally bound to both donors, the two lowest energy states being the symmetric and the antisymmetric combinations of the states $|A\rangle$ and $|B\rangle$ split by the energy $2W_{AB}$. In the opposite case of the strongly heteropolar donor pair with $|W_{AB}/\Delta| \ll 1$ the effect of the hopping interaction on energies and wavefunctions is strongly reduced: the electron is practically bound to one donor, the one with the lower external potential energy, V . The two donors forming a strongly heteropolar pair may be treated, to a good approximation, as single donors with purely electrostatic interaction. One can say that large enough potential energy differences, Δ , decouple donor pairs. Similar decoupling may be demonstrated for larger clusters: a triple may decouple into a pair and a single ion, or into three single ions, etc. Consequently, in weakly doped, strongly compensated semiconductors with their large potential energy fluctuations and large interdonor separations the electrons are in practice bound to the simplest ion clusters—in the first approximation to singles and pairs—with particularly low electronic potential energies due to the surrounding charged impurities. Of course, when one lets the number of electrons tend to zero as a result of more complete compensation, the rare clusters consisting of more very closely spaced donor ions come into play. The restriction it puts on compensation is difficult to specify but it is evidently much less severe here than in the model of pairs isolated from external fields exploited by Arendarchuk and co-workers [3].

In order to determine which pairs and single ions bind electrons we have to calculate the lowest energy states of our semiconductor. For each donor ion A we select the nearest neighbour B, assuming the Poisson distribution of impurities. Each donor having a negatively charged acceptor as the nearest neighbour is excluded from further considerations since its chances of binding an electron are very strongly reduced. Let r be the distance separating the donors A and B. We intend to treat the donor A with its nearest neighbour B as a pair, which interacts purely electrostatically with the random distribution of charges outside the sphere Q of radius r , centred at the donor A. Such a treatment is well justified for small r -values, but it meets difficulties with the increasing distance, r , to the nearest neighbour: the donor A is then not necessarily the nearest to its own nearest neighbour B, since the second neighbours to A are practically the same distance from A as the first one, etc. For this reason we introduce in our pair model a cut-off distance, r_0 . The atoms having nearest neighbours at distances exceeding r_0 will be treated as single ions interacting electrostatically with the charges outside the sphere Q_0 of radius r_0 . In selecting the value of r_0 we have to make a compromise: r_0 has to be large enough to justify neglecting the hopping integral W_{AB} and small enough to limit errors in the counting of pairs. The choice of r_0 will be discussed in the following.

In the description of random fields and potentials in strongly compensated materials we follow Morgan [4]. We approximate the probability distribution of the values V of the electron potential energy produced by impurities and electrons situated outside the sphere Q at the position of the donor A by the Gaussian distribution with zero average and root mean square value

$$\sigma = \sqrt{\langle V^2 \rangle} = E_1 a_B \sqrt{2\pi\lambda(N_D + N_A)} \exp(-r/\lambda) \quad (1)$$

where E_1 is the donor ionization energy, a_B is the effective Bohr radius. For the screening length λ we use the formula advocated in [1]:

$$\lambda = \mu(N_D + N_A)^{1/3} / (N_D - N_A)^{2/3}. \quad (2)$$

The numerical coefficient μ will be treated in the following as a variable parameter.

In calculating the energy spectrum and the wavefunctions of an electron localized at a donor pair we neglect the inhomogeneity of the external electric field in the region of the localization of the electron. We use different approximations for fields parallel, E_{\parallel} , and perpendicular, E_{\perp} , to the axis of the pair. For the field E_{\perp} we use the value at the centre of the sphere Q —each of the two cartesian coordinates having a normal distribution with a dispersion given by the formula

$$\sigma_{\perp}^2 = \sigma^2 \frac{2}{3e^2\lambda r} \left(1 + \frac{r}{2\lambda}\right) \quad (3)$$

and with zero mean value. For the field E_{\parallel} we use the value $-\Delta/er$ resulting from the value of the potential energy difference Δ between the two ionic positions A and B. Note that the potential energies at A and B are not independent random variables; for example, for very close ions the potential energies are practically equal. One can show, however, following Morgan's approach [4], that for a given distance r between the ions A and B the potential energy difference Δ has an approximately normal distribution, independent of the value of the potential energy V at the ion A but with dispersion σ_{Δ} dependent on the distance r :

$$\sigma_{\Delta}^2 = \sigma^2 \{1 - (2\lambda/r)\sinh(r/\lambda) + \frac{1}{2}\cosh(2r/\lambda) + (\lambda/4r)\sinh(2r/\lambda)[(2r/\lambda) + 1]\}. \quad (4)$$

For r tending to zero the dispersion σ_{Δ}^2 tends to zero as expected.

3. D_2^+ molecule in an electric field

The elementary LCAO model used above for qualitative considerations gives quite a good description of the two lowest states of an electron bound to a pair of donor ions (D_2^+ molecule) in the case of interdonor separations larger than about $5a_B$. The comparison of the predictions of this model with the exact calculations of Bates and co-workers [5] for a D_2^+ molecule without external fields clearly shows the inadequacy of the similar model for the excited states, even at quite large interdonor separations. For a better description of the energy spectrum and the wavefunctions of D_2^+ molecules in an external electric field we applied the exact wavefunctions of Bates and co-workers [5]. We selected the ten lowest energy states of the D_2^+ molecule (which for large interdonor separations tend asymptotically to 1s, 2s and 2p states of isolated atoms) and we diagonalized the Hamiltonian with the terms due to the uniform electric fields E_{\parallel} and E_{\perp} in the subspace spanned by the wavefunctions of these levels.

This procedure has an advantage over the standard perturbation approach, for its range of applicability extends to higher electric fields; even at quite high fields, which may occasionally occur in our model, the results are reasonable.

In constructing the secular equation we profited from the tabulated results of matrix elements of the dipole moment for the D_2^+ molecule [6]. The same tables were used later on to calculate the dipole transition rates for infrared absorption.

For the calculation of the Fermi energy one has to use the same energy scale for all pairs and single donors. For donors the distribution of the ground-state energies coincides to a good approximation with the distribution of potential energies V at the centre of the sphere Q_0 displaced by the ground-state energy $-E_1$ of an isolated donor. Thus the probability that an isolated donor is occupied is given by

$$\int_{-\infty}^{E_F + E_1} dV \exp(-V^2/2\sigma^2) / \sqrt{(2\pi)\sigma} = \text{FREQ}[(E_F + E_1)/2\sigma^2].$$

The Stark energy shifts of the ground donor states were found to be small at the scale of variations of V and they were neglected.

For donor pairs the ground-state energy was identified with the quantity $V + \Delta/2 + E_0(r, \Delta, E_{\perp})$, where $V + \Delta/2$ represents the random potential at the middle of the pair and $E_0(r, \Delta, E_{\perp})$ is the lowest energy state obtained by the diagonalization procedure for given values of E_{\perp} and $\Delta = -eE_{\parallel}r$. The probability of occupation of a pair is given by $\text{FREQ}\{[(E_F - \Delta/2 - E_0(r, \Delta, E_{\perp}))]/2\sigma^2\}$.

The Fermi energy was calculated numerically by equating the number of electronic ground states below E_F to the number of electrons $N_D - N_A$ per unit volume:

$$\begin{aligned} N_D [\exp[-x_0(1+K)] \text{FREQ}[(E_F + E_1)/\sigma] + \pi^{-1/2} \int_0^{x_0} dx \exp[-x(1+K)] \\ \times \int_{-\infty}^{\infty} dy \exp(-y^2) \int_0^{\infty} dz z \exp(-z^2) \text{FREQ}\{[E_F - 2^{-1/2}\sigma_{\Delta}y \\ - E_0(r_D x^{1/3}, 2^{1/2}\sigma_{\Delta}y, 2^{1/2}\sigma_{\perp}z)]/\sigma\}] = (1-K)N_D \end{aligned} \quad (5)$$

where $K = N_A/N_D$, $x = (r/r_D)^3$, $r_D = (3/4\pi N_D)^{1/3}$, $x_0 = (r_0/r_D)^3$, $y = 2^{-1/2}\Delta/\sigma_{\Delta}$, $z = 2^{-1/2}E_{\perp}/\sigma_{\perp}$. The first term represents the number of occupied donors with no neighbouring impurities closer than r_0 (as guaranteed by the exponential factor). The second term gives the number of singly occupied pairs of donor ions; for $N_D - N_A \ll N_D$ the

neutral donor pairs can be neglected. The occupation probability of a pair of donors, A and B, is integrated with the Gaussian distributions of transverse field E_{\perp} and the potential energy difference Δ and finally over all possible positions of donor B closest to donor A. Note that the temperature does not enter equation (5). This means that we limit our considerations to low temperatures with kT much smaller than the magnitude of typical fluctuations of the electron potential energy.

By repeating the calculations for different values of the cut-off distance, r_0 , we found that the value of E_F is only weakly affected by the errors in the counting of pairs with the largest interdonor separations. Consider, for example, the case of $N_D = 10^{15} \text{ cm}^{-3}$ ($r_D/a_B = 6.29$), $K = 0.94$, $\mu = \frac{1}{2}$. We obtained in this case $E_F = -2.05E_1$ for $r_0 = 4.5a_B$ and $E_F = -2.1E_1$ for $r_0 = 5.75a_B$. This change of the Fermi energy being an order of magnitude smaller than the typical potential energy fluctuations does not affect significantly the calculated absorption spectrum. Among the pairs which we add by increasing r_0 from $4.5a_B$ to $5.75a_B$ only two-thirds have the property that each ion is the nearest neighbour of the other; fortunately E_0 for most of the added pairs is much higher than E_F and the added pairs have little chance to be occupied. Consequently, their presence does not change significantly the occupation of pairs with smaller interdonor separations.

The Fermi energy E_F turns out to be very sensitive to the magnitude of the typical fluctuations. This becomes evident when we compare the values of E_F obtained for a given concentration and compensation but for different screening lengths—for $N_D = 10^{15} \text{ cm}^{-3}$ and $K = 0.94$ one gets $E_F = -2.1E_1$ for $\mu = \frac{1}{2}$ and $E_F = -3.4E_1$ for $\mu = 1$. In the model, neglecting all but the nearest neighbour interactions used by Arendarchuk and co-workers [3] one gets $E_F \approx -1.8E_1$ in this case. In general we found the downward shift of the Fermi energy due to fluctuating fields and potentials to be approximately equal to the dispersion of the potential energies.

4. Absorption coefficient

Once we have found the Fermi energy and we know how to calculate the energies and wavefunctions for the ground and the low-lying excited states of D_2^+ pairs in external electric fields, the calculation of the absorption coefficient due to these pairs is straightforward. We select all pairs having ground states below E_F which can absorb photons of a given energy. We calculate the oscillator strengths for the dipole optical transitions using the tables [6] and we perform the summation taking into account the statistical weight of absorbing pairs following the derivation of equation (5). Our final formula for the pair contribution to the absorption coefficient has the following form:

$$\begin{aligned} \alpha = & 3\pi^{1/2}\varepsilon^{-1}(e^2/\hbar c)r_D^{-3}\hbar\omega \sum_{j=1}^9 \int_0^{x_0} dx \exp[-x(1+K)] \\ & \times \int_{-\infty}^{+\infty} dy \exp(-y^2) \int_0^{\infty} dz z \exp(-z^2) |\langle \Psi_j | \mathbf{n} \cdot \mathbf{r} | \Psi_0 \rangle|^2 \\ & \times \text{FREQ}\{[E_F - 2^{-1/2}\sigma_{\Delta}y - E_0(r_D x^{1/3}, 2^{1/2}\sigma_{\Delta}y, 2^{1/2}\sigma_{\perp}z)]/\sigma\} \\ & \times \delta(z - z_{0j}) \left| \frac{\partial(E_j - E_0)}{\partial z} \right|^{-1}. \end{aligned} \quad (6)$$

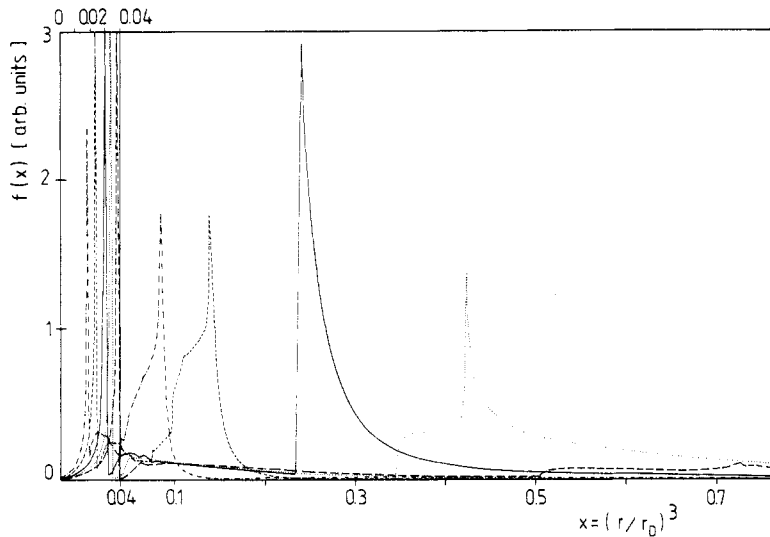


Figure 1. The absorption due to donor pairs D_2^+ as a function of the interdonor separation r for five different photon energies: $1.1 E_1$, $1.0 E_1$, $0.9 E_1$, $0.85 E_1$, $0.8 E_1$ (the spikes on the curves move to the right with increasing photon energy).

Most symbols used in the above equation have already been defined for equation (5). Besides those, ε is the dielectric constant, $\hbar\omega$ is the photon energy, Ψ_0 is the wavefunction of the ground state, Ψ_j and E_j are the wavefunction and the energy of the j th excited state ($j = 1, \dots, 9$), respectively. \mathbf{n} denotes the unit vector parallel to the electric field of the incident radiation, $e^2/\hbar c$ is the fine structure constant. Finally, z_{0j} are the solutions of the equations $E_j(z) - E_0(z) = \hbar\omega$, for $j = 1, \dots, 9$.

In equation (6) we did not include the transitions to high excited bound states and to continuum states of D_2^+ pairs. We observe however that all these transitions have low oscillator strengths, and that the weakly bound and continuum states are strongly affected by the random electric fields E_{\parallel} and E_{\perp} and also by the hopping interactions with more distant neighbours neglected in our model. We expect therefore that the absorption omitted in our calculations represents the structureless background slowly varying with photon energy.

Despite the presence of the Dirac δ -function none of the three integrations in (6) can be performed analytically. The zeros of the argument of the δ -function, as well as the derivative of this argument, have to be calculated numerically, a procedure involving the multiple solving of the secular 10×10 equation. The two remaining integrations are numerically quite complicated because of the behaviour of the integrand. In figure 1 we plotted the integrand of the integral over x for five different photon energies (with $N_D = 10^{15} \text{ cm}^{-3}$, $K = 0.94$, $\mu = \frac{1}{2}$, $r_0 = 5.75 a_B$). For each photon energy one can observe two spikes at the values of x close to the values expected for resonance pairs for the two lowest energy transitions. One can see, however, that in contrast to the model without the field and potential fluctuations, for each photon energy the pairs with a range of interdonor separations contribute to the absorption. It is particularly evident at low photon energies. Detailed analysis of the integrand of the internal integral shows that the spikes are due to the non-monotonic behaviour of certain transition energies with respect to the electric field. Qualitatively, this non-monotonic behaviour results from

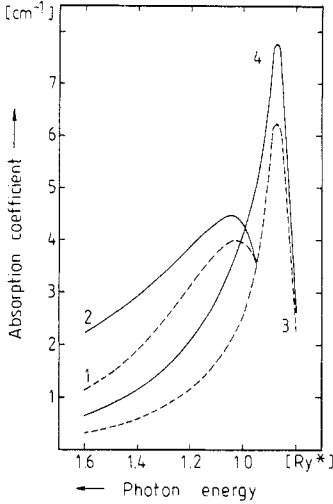


Figure 2. The pair absorption coefficient versus photon energy for n-type GaAs with $N_D - N_A = 3 \times 10^{13} \text{ cm}^{-3}$ electrons bound to donors and donor pairs. The four curves correspond to the following donor concentrations and screening uncertainty factors: 1. $N_D = 3 \times 10^{15} \text{ cm}^{-3}$, $\mu = 1$; 2. $N_D = 3 \times 10^{15} \text{ cm}^{-3}$, $\mu = \frac{1}{2}$; 3. $N_D = 1 \times 10^{15} \text{ cm}^{-3}$, $\mu = 1$; 4. $N_D = 1 \times 10^{15} \text{ cm}^{-3}$, $\mu = \frac{1}{2}$.

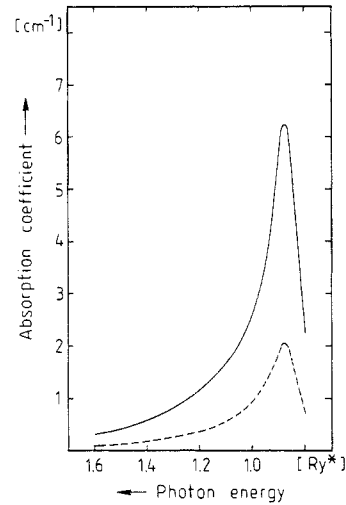


Figure 3. The pair absorption coefficient versus photon energy for n-type GaAs with the donor concentration $N_D = 1 \times 10^{15} \text{ cm}^{-3}$ and $\mu = 1$. The full curve corresponds to the compensation $K = 0.94$, the broken one to $K = 0.98$.

the competition between the linear and the quadratic Stark effect for the two levels involved in the transition.

The behaviour of the integrand in figure 1 indicates that for donor concentrations of $1 \times 10^{15} \text{ cm}^{-3}$ and all higher concentrations our results for the lowest photon energies are rather approximate. The important part of the absorption at these energies comes from the pairs with large interdonor separations for which the pair model is not quite adequate.

5. Results and discussion

In figure 2 we present the pair contribution to the absorption coefficient calculated for n-type GaAs for two concentrations of shallow donors $N_D = 1 \times 10^{15} \text{ cm}^{-3}$ and $N_D = 3 \times 10^{15} \text{ cm}^{-3}$. For still higher concentrations the pair model is questionable, for lower concentrations the calculated absorption coefficients are rather low. In a preliminary report of our results [7] we presented the absorption coefficient for the higher concentration ($N_D = 3 \times 10^{15} \text{ cm}^{-3}$) in the more extended range of photon energies. In the subsequent analysis we found that for photon energies smaller than about E_1 the absorption calculated for this concentration comes predominantly from pairs with the interdonor separations close to the cut-off distance r_0 and that at these energies the results are r_0 -dependent and thus not reliable. The photon energy below which the results exhibit significant dependence on r_0 is concentration-dependent, since r_0 itself

depends on concentration. At low concentration larger r_0 might be chosen, and the calculated absorption remains independent of r_0 down to lower photon energies.

All curves presented in figure 2 correspond to the same number of electrons, $N_D - N_A = 6 \times 10^{13} \text{ cm}^{-3}$, sitting on donors and donor pairs, the compensation K being equal to 0.94 and 0.98 for the lower and the higher concentration of donors, respectively. For both concentrations we selected two different screening regimes: $\mu = 1$ and $\mu = \frac{1}{20}$ for the lower, and $\mu = 1$ and $\mu = \frac{1}{7}$ for the higher donor concentration.

One can see that in all cases the pair absorption exhibits a maximum shifted towards higher frequencies when compared with the 1s–2p transition for isolated donors, the shift being larger for larger concentrations. This effect is qualitatively the same as that discussed by Arendarchuk and co-workers [3]: namely, for higher donor concentrations more pairs with small interdonor separations are populated (when the number of electrons is kept constant). In contrast to Arendarchuk and co-workers [3] we do not find, however, the quantitative coincidence between the energy of the maximum and the transition energy for the resonance pairs with the ground states just at the Fermi energy.

Comparison between the curves corresponding to the same donor concentration (curves 1 and 2 or 3 and 4 in figure 2) indicates that the increase in magnitude of fluctuations when passing from more to less effective screening (from smaller to larger μ) consists of the decrease of the pair absorption, in particular at high photon energies. As a result of the increasing potential energy fluctuations some pairs with small interdonor separations absorbing at high photon energy lose their electrons producing more numerous pairs with larger donor separations and more isolated donors which may occasionally have very low potential energies V .

In figure 3 we compared the results obtained for one given donor concentration, $N_D = 1 \times 10^{15} \text{ cm}^{-3}$, and the same screening regime $\mu = 1$ but with electron concentrations differing by a factor of 3: $K = 0.94$ and $K = 0.98$. Even though the Fermi energies in both cases are quite different ($-1.72E_1$ and $-3.06E_1$, respectively) the absorption turns out to scale almost linearly with $1 - K$. The absorption for the higher electron concentration is practically equal to that for the lower concentration multiplied by a factor 3.

In general one can say that the pair contribution represents significant absorption in the spectral region above the 1s–2p transitions of isolated donors, with a specific dependence on donor concentration and compensation and on the magnitude of the field and the potential fluctuations.

The results of the present paper suggest that the ‘deeper donors’ observed by Paget and Klein [2] in compensated n-type GaAs should be identified with charged donor pairs D_2^+ with different interdonor separations. Our results seem to indicate that careful experimental studies of the evolution of the far infrared absorption spectra with impurity concentration and compensation may furnish information on the magnitude of the potential energy fluctuations in strongly compensated semiconductors. In particular the data of Arendarchuk and co-workers [3] suggest that in n-type InSb either the screening is more effective than it might seem from theoretical estimates or that the charged impurities are not randomly distributed.

References

- [1] Shklovsky B I and Efros A L 1984 *Electronic Properties of Doped Semiconductors* (New York: Springer)

- [2] Paget D and Klein P B 1986 *Phys. Rev. B* **34** 971
- [3] Arendarchuk W W, Gershenzon E M, Litvak-Gorskaja L B and Rabinovich R J 1973 *Zh. Eksp. Teor. Fiz.* **6** 2387 (Engl. Transl. 1974 *Sov. Phys.-JETP* **38** 1192)
- [4] Morgan T N 1965 *Phys. Rev. A* **139** 343
- [5] Bates D R, Ledsham K and Stewart A L 1953 *Phil. Trans. R. Soc. London A* **246** 215
- [6] Ramaker D E and Peek J M 1973 *Atom. Data* **5** 167
- [7] Blinowski J and Szwacka T 1990 *Acta Phys. Pol. A* **77** 55