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Capture of carriers by screened charged centres and low-temperature shallow-impurity electric field breakdown in semiconductors

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Abstract. Free-carrier capture by a screened Coulomb potential in a semiconductor is considered. It is established that with decreasing screening radius the capture cross section decreases drastically, and it goes to zero when $r_s = a_B^*$. On the basis of this result, a new mechanism of shallow-impurity electric field breakdown in semiconductors is suggested.

1. Introduction

For correct consideration of the kinetic, photoelectrical and optical phenomena in semiconductors and semiconductor structures, it is necessary to take into account the carrier capture by attractive centres. Among these centres in semiconductors are negatively or positively charged shallow acceptors or donors, whose potential is usually considered as a Coulomb interaction. The capture of carriers by a Coulomb centre in a semiconductor was first considered by Lax [1] and a corrected version of this work was given in [2]. In [2], the capture theory was developed for small and large concentrations of impurities. In the first case, the capture occurs at isolated centres. In the second case, which is characterized by an overlap of the effective capture orbits ($r_T = e^2/\chi kT$) of neighbouring centres, it was supposed that the capture takes place in the wells of the potential fluctuations of the impurities. This gives an essentially weak dependence of the capture cross section (CCS) on the centre concentration ($\sigma \sim N_d^{1/6}$) compared with that for isolated centres ($\sigma \sim N_d$). However, the potential of the charged impurity in real semiconductors may be considered as purely Coulombic in the weak-doping case only ($N_d^{1/3} a_B^* \ll 1$, where N_d is the shallow-impurity concentration and a_B^* is the effective Bohr radius). With increasing impurity concentration, the potential of the charged centre changes from a Coulomb- to a Yukawa-type potential as a result of the screening by free electrons and charged impurities.

In this work we will consider the capture process in the case of a high free-carrier concentration n, for which Debye screening of a Coulomb centre occurs. Such a situation can be realized in semiconductors in the following circumstances.

(i) In the case of high impurity concentration and at relatively high temperatures when kT is comparable with the shallow-impurity ionization energy ϵ_i, with the result that most of the shallow impurities are ionized ($n \sim N_d$).

(ii) In the case of small as well as high concentrations of impurities and low temperatures ($kT \ll \epsilon_i$), if a sufficiently strong electric field is applied to the semiconductor. As is known

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[2, 3], the CCS would decrease under the electric field, and as a result the free-electron concentration would increase [4]. As will be shown, for the case of strong free-electron screening the CCS goes to zero.

2. The capture cross section for a screened Coulomb centre

We consider the capture of free carriers by a potential of the form

$$U = -(e/\chi r)\exp(-r/r_s). \tag{1}$$

In (1), r_s is the Debye screening radius, and it must be chosen as

$$r_s = \chi E_F/(6\pi n e^2)$$

in the degenerate case and as

$$r_s = \sqrt{\chi kT/(4\pi n e^2)}$$

in the nondegenerate case, where $E_F = h^2k_F^2/2m^*$, $k_F = (4\pi n^2)^{1/3}$, χ is the dielectric constant and n is the free-carrier concentration. Note that in the conduction band bottom of gap semiconductors, the carrier distribution can be taken as a Boltzmann one in the low-temperature and high-concentration case.

Like in the Coulomb potential case, the effective capture radius for the centre is determined from the equation

$$E = (e^2/\chi r)\exp(-r/r_s) \tag{2}$$

where E is the total energy of the carriers. In contrast to the Coulomb potential case, equation (2) is transcendental, and cannot be solved analytically.

To calculate the CCS we use the following expression [2]:

$$\sigma = [(\pi h)^2/(2kTm^\star)]\left[\int_{-\infty}^{0}\exp(E/kT)B^{-1}(E)\ \mathrm{d}E\right]^{-1} \tag{3}$$

where

$$B(E) = \int \epsilon\tau^{-1}(\epsilon)\rho(\epsilon)\delta[E-\epsilon-U(r)]\ \mathrm{d}\epsilon\ \mathrm{d}^3r \tag{4}$$

with

$$\begin{aligned}\rho(\epsilon) &= 8\sqrt{2}\pi(2\pi h)^{-3}m^{\star 3/2}\epsilon^{1/2}\\ \tau(\epsilon) &= l_0(m^\star/(2\epsilon))^{1/2}\\ l_0 &= (\pi h^4\rho_0)/(2m^{\star 3}E_c^2).\end{aligned} \tag{5}$$

E_c is the deformation potential constant, ρ_0 is the crystal density and $m^\star$ is the carrier effective mass. At low temperatures, electrons are distributed between the impurity ground state 1s and the conduction band bottom. In such a situation, carriers cannot be captured by emission of optical phonons because their energy is greater than the distances between the shallow-impurity states (at least for most semiconductors). For this reason, formula (3) describes capture owing to diffusion lowering of carriers as a result of their wandering between excited states of the impurity by means of absorption or emission of acoustic phonons only.

Substituting (1) and (5) into (4) and after integrating using δ-function properties, it is easy to obtain for $B(E)$ the expression

$$B(E) = [8m^\star/(\pi l_0 h^3)]\left[\frac{1}{3}E^2 r_i^3 + 2E^2 r_i r_s^2\left(1 + \frac{r_i}{r_s} - \mathrm{e}^{r_i/r_s}\right) + \frac{1}{2}E^2 r_i^2 r_s(\mathrm{e}^{r_i/r_s} - 1)\mathrm{e}^{r_i/r_s}\right]. \tag{6}$$

The expression for $B(E)$ can be written in the form

$$B(E) = [8m^\star/(\pi l_0 h^3)](r_s^3 E^2/6)J(x) \tag{7}$$

where

$$J(x) = 2x^2 + 12x(1 + x - \exp(-x)) + 3x^2(\exp(x) - 1)\exp(x) \tag{8}$$

where $x = r_i/r_s$ and r_i is the root of equation (2) for a given screening length r_s. Note that in obtaining (6) and (7) for each r_s, we first find r_i numerically from (2), and then substitute this value in as an upper limit of the integral (4).

Substituting (6) and (7) into (3), we obtain an expression for the CCS:

$$\frac{\sigma_0}{\sigma} = [2/(kT)^2](e^2/\chi r_s)^3 \int_0^\infty \exp(-E/kT)/(E^2 J(x))\ \mathrm{d}E \tag{9}$$

where

$$\sigma_0 = (4\pi/3l_0)(e^2/\chi kT)$$

is the CCS in the Coulomb potential case.

The results of numerical calculation of the dependence of σ_0/σ on r_s/a_B^* at $T = 4.2$ K for GaAs (curve 1) and Ge (curve 2) with the parameters $m^\star = 0.067m$, $\chi = 12.5$ and $m^\star = 0.082m_0$, $\chi = 16$, respectively, are shown in figure 1.

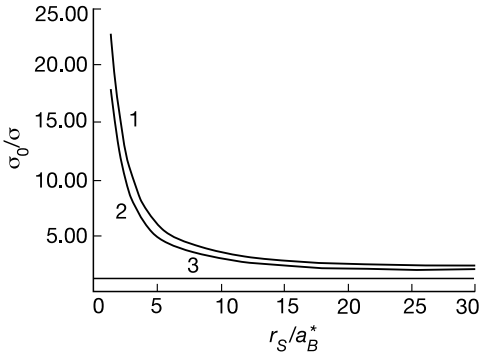

Figure 1. The dependence of σ_0/σ on the screening radius r_s/a_B^* for GaAs (curve 1), for Ge (curve 2) and in the Coulomb potential case (curve 3).

It is easy to show that when $r \to \infty$ for the CCS from equation (8), the Coulomb potential case is obtained. Note that the screened potential (1), in contrast to the Coulomb one, has a finite number of bound states, and when $r \leqslant a_B^\star$ has no bound states at all they merge into the continuous bands [5, 6]. It is obvious that, in the absence of bound states, the CCS must be equal to zero for such a centre. But as is seen from figure 1, when $r_s = a_B^\star$ the CCS—unlike that in the Coulomb potential case—decreases by factors no larger than 20 and 25 for Ge and GaAs respectively. This means that the diffusive method used for the

CCS calculation in [2] and in this work becomes inapplicable at small screening lengths, when the number of discrete states is small. In this case the capture process cannot be considered as a diffusive lowering of carriers through energetic states of the impurity. Note that, owing to this, the values of σ_0/σ would be higher than those represented by curves 2 and 3 not just for $r_s = a_B^\star$.

Thus we obtain the simple result that the greater the degree of screening, the lower the capture coefficient—and when $r_s = a_B^\star$, it is equal to zero. It is obvious that the analogous result must be obtained for the coefficient of thermal ionization from impurity states because of the lowering of the ionization energy ϵ_i from these states when the screening is strong (the ionization probability $w_i \sim \exp(-\epsilon_i/kT)$). Now we will consider some consequences of the result obtained.

3. The low-temperature shallow-impurity electric field breakdown mechanism

We will discuss the low-temperature shallow-impurity electric field breakdown (the LTSIEFB) phenomenon for semiconductors. From the first observations of LTSIEFB [7] up to the present [8], it has been believed that this phenomenon is just due to impact ionization of neutral impurities by free electrons as a result of their heating under an external electric field. Our result allows us to put forward an alternative mechanism for LTSIEFB, which explains all of the peculiarities of the current–voltage characteristics (CVC) of semiconductors, including the avalanche-like increase of the current and the S-like form of the CVC at the breakdown electric field. According to this mechanism, with increasing electric field the concentration of the free carriers n will increase, because of the well known decrease of the capture coefficient α and the increase of the ionization coefficient β. The value of n in an electric field would be established by the condition of balance between the capture and thermic ionization, $n\alpha N_D^+ = \beta N_D^0$ (N_D^0 is the neutral-donor concentration and $N_D^+ = N_A + n$ is the charged-donor concentration):

$$n(\mathcal{E}) = [N_D^0(\mathcal{E})/N_D^+(\mathcal{E})]\beta(\mathcal{E})/\alpha(\mathcal{E}). \tag{10}$$

At some electric field, which is very close to the breakdown one, the value of n would be so high that screening of the charged impurities would occur. At this instant, an avalanche increase of the free-carrier concentration will begin, owing to the decrease of the CCS because of screening and, as a result of this, a further increase of $n(\mathcal{E})$, and so on. Thus the dependencies $n(\mathcal{E})$ and

$$j(\mathcal{E}) = en(\mathcal{E})\mu(\mathcal{E})\mathcal{E} \tag{11}$$

will show an avalanche-like increase with electric field. Note that LTSIEFB takes place at low temperatures when the dominant scattering mechanism of the carriers is that by charged impurities. This means that, owing to the screening of charged-impurity potentials, the mobility of the carriers $\mu(\mathcal{E})$ at the breakdown electric field will increase, and as a result of this the CVC will have an S-like character. Screening-induced increase of $\mu(\mathcal{E})$ causes an additional (besides that of $n(\mathcal{E})$) current increase in the avalanche-like region of the CVC. Note that it was already established from cyclotron resonance line-shape investigations of n-GaAs that free-carrier screening of charged impurities is strong at the breakdown electric fields [9, 10]. For LTSIEFB there is no need for the condition $r_s = a_B^*$ to be obeyed, when total screening of the impurity state occurs. First of all, such a condition means that all neutral shallow impurities have to be ionized in semiconductors. But, as was shown from Hall measurements [11] at the breakdown electric field for n-Ge, only 5% and, from the plasma shift of the cyclotron resonance line for n-GaAs [12] at electric fields three

times the breakdown one, only about 40% of the neutral impurities were ionized. On the other hand, the condition $r_s = a_B^*$ also corresponds to a Mott transition which occurs at sufficiently high impurity concentrations, $-N_D^{1/3} a_B^* \approx 0.25$, and in this case all impurity electrons are in the conduction band [13]. Hence LTSIEFB must discontinue at very high impurity concentrations. Note that, according to the screening mechanism of LTSIEFB, it must disappear in the low-impurity-concentration case too, as can be determined from the condition $r_s = r_T = e^2/\chi kT$. Consequently, according to the supposed mechanism, LTSIEFB takes place only at neutral-impurity concentrations

$$(\chi kT/e^2)^3(1/4\pi) < N_D^0 < (0.25/a_B^*)^3.$$

For n-GaAs, this condition requires

$$5 \times 10^{11}\ \mathrm{cm}^{-3} < N_D^0 < 2 \times 10^{16}\ \mathrm{cm}^{-3}.$$

In another article, I will present experimental evidence which contradicts the impact ionization model and confirms the above mechanism for LTSIEFB in n-GaAs. The fact that the CCS goes to zero when $r_s \leqslant a_B^*$ may be considered as one of the reasons for a Mott transition occurring in semiconductors.

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References

[1] Lax M 1960 *Phys. Rev.* **9** 1502
[2] Abakumov V N, Perel V I and Yassievich I N 1978 *Fiz. Tekh. Poluprov.* **12** 3
See also:
Abakumov V N *et al* 1991 *Non-radiative Recombination in Semiconductors* (Oxford: North-Holland)
[3] Godik E E, Kuritchin Y A and Sinis V P 1978 *Fiz. Tekh. Poluprov.* **12** 351
[4] Alekperov O Z 1988 *Reports of the Scientific and Industrial Association for Space Research (Baku)* pp 230–5
[5] Rogers F J, Craboske H C and Harwood D Y 1970 *Phys. Rev.* A **1** 1577
[6] Flugge S 1974 *Practical Quantum Mechanics I* (Moscow: Nauka) p 341
[7] Koenig S H and Gunther-Mohr G R 1957 *J. Phys. Chem. Solids* **2** 268
[8] Sablikov V A, Polyakov S V and Ryabushkin O A 1996 *Fiz. Tekh. Poluprov.* **30** 1251
[9] Alekperov O Z, Golubev V G and Ivanov-Omskii V I 1983 *Fiz. Tekh. Poluprov.* **17** 155
[10] Alekperov O Z, Golubev V G, Ivanov-Omskii V I and Mekhtiev A Sh 1983 *Phys. Status Solidi* b **120** K179
[11] Zavaritskaya E I 1966 *Trudy Fiz. Inst. P N Lebedeva Akad. Nauk SSSR* **37** 41
[12] Alekperov O Z, Golubev V G, Ivanov-Omskii V I and Mekhtiev A Sh 1985 *Phys. Status Solidi* b **127** K171
[13] Mott N F and Davis E A 1982 *Electron Processes in Non-crystalline Materials* vol 1 (Moscow: Nauka) p 368