



Charged impurity scattering of electrons in quasi-two dimensional semiconductor systems

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In this paper the dependencies between the relaxation period of electrons and the energy of mobility and temperature in a quasi-two dimensional, nondegenerate semiconductor nanostructure, using a common model of the admixture centre, are calculated. The electrons' relaxation period and their mobility depend on the depth of the nanostructure, and even more upon the radius of the short-range potential influence (first coordination sphere radius). Moreover, the electron relaxation time $\tau(\epsilon) \sim \epsilon$ and mobility $\mu(kT) \sim (k_B T)$, and a formula is derived for the thermal electromotive force of this system.

The problem of the dispersion (scattering) of electrons in ionized admixtures (charged impurities) in semiconductor crystals in a 3D system was solved by Conwell–Weisskopf [1] and then by Brooks–Herring who took into consideration the process of screening by impurity centres [1]. They considered the centre of the impurity potential using a Coulomb approximation and determined the dependency between the electrons' relaxation time and energy: $\tau(\epsilon) \sim \epsilon^{3/2}$. This is the “three seconds” rule, where $\tau(\epsilon)$ is the electron relaxation time and ϵ is the electron energy. It turns out that in the case of comparatively high temperature and concentration, dominated by dispersion in ionized admixtures, that the results of their method are quite different from experimental results [2, 3]. Unfortunately, the theory ignores the type of the admixture, although in experiments its dependency is observed [4].

A group of authors (A. Gerasimov, Z. Gogua and A. Tsertsvadze) have postulated a common model of the impurity centre [5], whereby the first coordination sphere is considered as a free atom in vacuum, and outside (as usual) is the continuum approximation. According to this model, the potential of the impurity centre is:

$$\phi(r) = \frac{z^*e}{r} \theta(r - r_0) + \frac{ze}{\epsilon_0 r} \theta(r - r_0), \quad (1)$$

where z^* is the impurity atom effective charge, z the impurity atom charge in the continuum approximation, r_0 the radius of the first coordination sphere, ϵ_0 the permittivity of free space and

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$\theta(x)$ the Heaviside step-function. The effective charge of the impurity atom can be defined using Slater's free atom model [7]:

$$z^* = n^* \sqrt{\frac{I}{E_H}}, \quad (2)$$

where I is the first ionization energy. E_H is the absolute value of the ground state energy of the free hydrogen atom, n^* is the principal quantum number, which is defined using Slater's rule [7], hence z^* represents the individuality of the atom. With this approach, the problem of expressing deep and shallow impurity levels with one common model is solved [5]. The problem of emitting and nonemitting dispersion of charge carriers at impurity centres [8, 9] and the problem of the dispersion of electrons at impurity centres for the potential when $z = 1$, can be obtained by solving Poisson's equation. Hence, the shielded potential of the impurity centre [6] is:

$$\phi(r) = \frac{z^* e}{r} \theta(r - r_0) + \frac{e}{\epsilon_0 r} e^{-qr} \theta(r - r_0), \quad (3)$$

where q is the inverse Debye radius. Using this potential, in the case of a nondegenerate electron gas, it is possible to calculate the relaxation time and mobility of the electrons. When the influence of the inner potential of the impurity centre is highly increasing:

$$4 \left(\frac{z^* \epsilon_0}{z} \right) \left(\frac{r_0}{a_0} \right)^2 \left(\frac{m^*}{m} \right) \left(\frac{\epsilon}{E_H} \right) \gg 1, \quad (4)$$

where m^* is the electron effective mass and m is the free electron mass. In the Born approximation this gives:

$$\tau(\epsilon) = \frac{\sqrt{2}}{4\pi} \frac{\epsilon_0 m E_H}{z^* e^4 \sqrt{m^* n_i}} \left(\frac{a_0}{r_0} \right)^2 \epsilon^{1/2} \sim \epsilon^{1/2} \quad (5)$$

and

$$\mu = \frac{\sqrt{2} \epsilon_0 \hbar^2}{3 \sqrt{(\pi m^*)^3} z^* n_i e^2 r_0^2} (k_B T)^{1/2} \sim (k_B T)^{1/2} \quad (6)$$

where a_0 is the Bohr radius of the hydrogen atom, n_i is the concentration of ions in the given material and k_B is Boltzmann's constant.

So, the "three seconds" rule becomes "one second". Equations (5) and (6) show that from condition (4) the calculation of relaxation period and mobility are dominated by the potential of the impurity centre (the first part of equation 3). Physically, it means, that condition (4) is realized where the temperature is high and where the concentration of the admixture is also rather high, then dispersion at the ionized impurity will dominate. In these conditions the de Broglie wavelength of the electrons decreases and in the part of the region where the potential of the impurity centre is defined, r_0/λ increases. Thus, this region becomes more sensitive. The results of calculations using equations (5) and (6) are rather closer to the experimental data than the results of Conwell–Weisskopf and Brooks–Herring [6]. In

nanostructures, (quasi-two dimensional semiconductor structures) our model of the impurity centre 3D system will work better, because in flat nanostructures there is a defined region that is consistent with the zone where the impurity potential is much larger than in the continuum approximation. References [10–12] show that it is ineffective to use the continuum approximation when solving dispersion problems, and the authors consider the Coulomb potential at the impurity centre as a short-range potential.

This model has been applied in solving the problem of the ionization energy of a donor impurity in quantum wires [13].

If we have quasi-two dimensional system (i.e., a flat nanostructure) with depth W , then equation (3) for the potential in polar coordinates will be:

$$\varphi(\rho, z) = \frac{z^* e}{\sqrt{\rho^2 + z^2}} \theta(r_0 - \rho) \theta(r_0 - z) + \frac{e}{\epsilon_0 \sqrt{\rho^2 + z^2}} e^{-q\sqrt{\rho^2 + z^2}} \theta(\rho - r_0) \theta(z - r_0). \quad (7)$$

In a given quasi-two dimensional system, the Bloch function of a quasifree electron looks like [10, 12]:

$$\Psi(r, z) = \sqrt{\frac{2}{SW}} \sin\left(\frac{\pi z}{W}\right) e^{-i\vec{k}_\parallel \vec{\rho}} U_{\vec{k}_\parallel}(\vec{\rho}, z), \quad (8)$$

where S is the area of the structure, $\vec{k}_\parallel$ is the component of impulse on the Slater parallel plane and $U_{\vec{k}_\parallel}(\vec{\rho}, z)$ is Bloch's modulating factor. Our calculation of $\tau(\epsilon)$ is based not on the results in ref. 10, but by considering that the potential used at the impurity centre is a short-range potential; then the correspondence of relaxation periods in the cases of 2D and 3D systems is independent of the type of potential. It equals:

$$\frac{\tau_{2D}(\epsilon)}{\tau_{3D}(\epsilon)} = \frac{2k_W}{3\pi}, \quad (9)$$

where k is the wave vector of the electrons in the 3D systems:

$$k = \sqrt{\frac{2m^*}{\hbar^2} \epsilon}. \quad (10)$$

Based on this and the formula for $\tau_{3D}(\epsilon)$, equation (5), we get:

$$\tau_{2D}(\epsilon) = \frac{1}{6\pi^2} \frac{\epsilon_0 m^2 W}{z^* \hbar^3 n_I} \left(\frac{a_0}{r_0}\right)^2 \epsilon \sim \epsilon. \quad (11)$$

Therefore the electron relaxation time depends on the depth W of the structure and on the radius of the area of influence of the inner potential (first part of equation 3).

In the case of a quasi-two dimensional system, the electrons mobility with a nondegenerate electron system, based on [10] and [14] suggests:

$$\mu_{2D}(kT) = \frac{2e}{3m^*(k_B T)^2} \int_0^\infty \tau_{2D}(\epsilon) \epsilon e^{-\frac{\epsilon}{k_B T}} d\epsilon. \quad (12)$$

If we add equation (11) to this expression we obtain:

$$\mu_{2D}(kT) = \frac{5e\epsilon_0 m^2}{9\pi^2 m^* z^* \hbar^3 n_I} w \left(\frac{a_0}{r_0} \right) (k_B T) \sim (k_B T). \quad (13)$$

The mobility of a 2D electron gas, during dispersion in correlated distributed admixtures of quasi-two dimensional GaAs is directly proportional to temperature [15–17]. And for quasi-two dimensional systems the thermal electromotive force will be [11]:

$$\alpha_{2D}(T) = \frac{\pi^2}{3} \left(\frac{k_B}{e} \right) \left(\frac{k_B T}{E_F} \right) \left(1 + E_F \frac{\partial \ln \tau_{2D}(\epsilon)}{\partial \epsilon} \right)_{\epsilon=E_F}, \quad (14)$$

where E_F is the Fermi energy. Based on equation (11)

$$\left(1 + E_F \frac{\partial \ln \tau_{2D}(\epsilon)}{\partial \epsilon} \right)_{\epsilon=E_F} = 2, \quad (15)$$

so that

$$\alpha_{2D}(T) = \frac{2\pi^2}{3} \left(\frac{k_B}{e} \right) \left(\frac{k_B T}{E_F} \right), \quad (16)$$

which relies upon Heisenberg's condition of using the kinetic equation $\tau(\epsilon) \gg \frac{\hbar}{\epsilon}$, and implies that:

$$w \gg \frac{6\pi^2 z^* \hbar^4 n_I}{\epsilon_0 m^2} \left(\frac{r_0}{a_0} \right)^2 \frac{1}{(k_B T)^2}. \quad (17)$$

If we consider a nondegenerate crystal heavily doped with shallow impurities of Ge and Si, with $n_I \sim 3 \times 10^{18} \text{ cm}^{-3}$, at room temperature then dispersion dominates in the ionized admixture [2]. That means that $w \gg 2\text{--}3 \text{ nm}$.

Our results show the dependence on impurity type as represented by the effective main quantum number n^* and with the ionization energy of the electrons (first ionization energy).

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