საქართველოს მეცნიერებათა ეროვნული აკადემიის მოამბე, ტ. 3, №1, 2009
BULLETIN OF THE GEORGIAN NATIONAL ACADEMY OF SCIENCES, vol. 3, no. 1, 2009

Physics

Dispersion of Electrons on Ionized Admixtures in Semiconductors in Quasi-Two-Dimensional Systems

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(Presented by Academy Member G. Chagelishvili)

ABSTRACT. In this paper the dependences are calculated between the relaxation period of electrons and energy and between mobility and temperature in quasi-two-dimensional, non-degenerated semiconductor nanostructures, using the common model of admixture center. It is shown that the relaxation period of electrons and their mobility depends on the depth of nanostructure, and even greater on the radius of short-range potential influence (first coordination sphere radius). It is shown also that the relaxation period of electrons is $\tau(\varepsilon) \sim \varepsilon$ and mobility - μ *(KT)~(KT)*. The thermal electromotive force for this system is calculated. *© 2009 Bull. Georg. Natl. Acad. Sci.*

Key words: *dispersion, mobility.*

The problem of dispersion of electrons on ionized admixtures in semiconductor crystals in 3D system was solved by Conwell-Weisskopf [1] and then by Brooks-Herring [1]. They considered the potential of impurity center using Coulomb approximation and they got the same result for the dependence between electrons' relaxation and energy: $\tau(\varepsilon) \sim \varepsilon^{3/2}$. It is the rule of "three seconds", where $\tau(\varepsilon)$ is an electron's relaxation period and ε is an electron's energy. It turns out that in the case of comparatively high temperature and concentration, when dispersion on ionized admixtures still dominates, the results of their method are quite different (1-1.5 degrees) from experimental results [2, 3]. Besides, this theory does not show the individuality of admixture, though it is well-reflected in experiments [4].

A group of authors (A. Gerasimov, Z. Gogua, and A. Tsertsvadze) offered a general model of impurity center [5]. According to it, impurity center in the first coordination sphere is considered to be a free atom in vacuum, and outside of it to be usual, in continuum approximation. According to this model the potential of the impurity center will be:

$$\varphi(r) = \frac{z^* e}{r}\theta(r - r_0) + \frac{ze}{\varepsilon_0 r}\theta(r - r_0). \qquad (1)$$

Here z^* is impurity atom's effective charge, z - impurity atom's charge in continuum approximation, r_0 is radius of the first coordination sphere, ε_0 is the dielectric constant, $\theta(x)$ is step function of Heavyside. The effective charge of an impurity atom can be defined using Slater's free atom model [7]: $z^* = n^* \sqrt{\frac{I}{E_H}}$, where I is the first ionization energy of impurity atom, E_H is the absolute value of basic state energy of free hydrogen atom, n^* is the main quantum number, which is defined using Slater's rule [7]. z^* shows us the individuality of atom. Owing to this model, the problem of expressing deep

and shallow impurity levels with one, common model is solved [5]. The problem of emitting and non-emitting dispersion of charge careers on impurity centers [8, 9] and the problem of dispersion of electrons on impurity centers for (1) potential, when z=1, can be worked out by solving Poisson's equation. So, we shall get the shielded potential of impurity center [6]:

$$\varphi(r)=\frac{z^*e}{r}\theta(r-r_0)+\frac{e}{\varepsilon_0 r}e^{-qr}\theta(r-r_0), \qquad (2)$$

where q is the inverted value of Debye's radius. Using this potential, in the case of non-degenerated electron gas, it is possible to calculate the relaxation period and mobility of an electron. When

$$4\left(\frac{z^*\varepsilon_0}{z}\right)\left(\frac{r_0}{a_0}\right)^2\left(\frac{m^*}{m}\right)\left(\frac{\varepsilon}{E_H}\right)>>1. \qquad (3)$$

Here m^* is the electron's effective mass, and m is free electron's mass. In Borne approximation we shall get:

$$\tau(\varepsilon)=\frac{\sqrt{2}}{4\pi}\frac{\varepsilon_0 m E_H}{z^*e^4\sqrt{m^*}n_I}\left(\frac{a_0}{r_0}\right)^2\varepsilon^{1/2}\sim\varepsilon^{1/2}, \qquad (4)$$

$$\mu=\frac{\sqrt{2}\varepsilon_0\hbar^2}{3\sqrt{(\pi m^*)^3}z^*n_I e^2 r_0^2}(k_0T)^{1/2}\sim(k_0T)^{1/2}, \qquad (5)$$

where a_0 is Bohr radius in hydrogen atom, n_i is concentration of ions in given material and k_0 is Boltzman constant. So, the rule of "three seconds" turns into the rule of "one second". As (4) and (5) formulas show, realizing (3) condition, in calculation of relaxation period and mobility of atom, the main role is played by the potential of impurity center (1st part of (2) potential). Physically, it means that (3) condition is realized in high temperature range and if the concentration of admixture is rather high, then dispersion on ionized impurity will be more dominating than other mechanisms. In these conditions de Broglie's wave length of electron decreases and part of the area, where the potential of impurity center is defined $\left(\frac{r_0}{\lambda}\right)$, increases. So, this area becomes more "sensitive". The results of calculations using (4) and (5) formulas are rather closer to experimental data than Conwell-Weisskopf's and Brooks-Herring's theories [6]. In nanostructures, (quasi-two-dimensional semiconductor structures) it is logical to operate using our model of impurity center than in 3D systems, because in flat nanostructures there is a definite area which is consistent with the area where the impurity potential is much greater than in continuum approximation. In papers [10-12] is shown, that it is not effective to use continuum approximation when we are solving dispersion problems and authors consider the potential of impurity center as short-range potential.

Besides, we must say modestly that the author of paper [13] points to operate using this model in solving the problem of ionization energy of donor impurity, which is located in quantum wires.

If we have a quasi-two-dimensional system (flat nanostructure) with W depth, then (2) potential in polar coordinates will be:

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

$$+\frac{e}{\varepsilon_0\sqrt{\rho^2+z^2}}e^{-q\sqrt{\rho^2+z^2}}\theta(\rho-r_0)\theta(z-r_0) \qquad (6)$$

In the given quasi-two-dimensional system, Bloch's function of quasi-free electron looks like this [10, 12]:

$$\Psi(r,z)=\sqrt{\frac{2}{SW}}\sin\left(\frac{\pi z}{W}\right)e^{-i\vec{K}_{II}\vec{\rho}}U_{\vec{k}_{II}}(\vec{\rho},z), \qquad (7)$$

where S is area of structure, $\vec{k}_{II}$ is component of impulse on Slater's parallel plane and $U_{\vec{k}_{II}}(\vec{\rho},z)$ is Bloch's modulating factor. Our calculation of $\tau(\varepsilon)$ is based not on the usual method, but on results in paper [10], where it is said that if we consider the potential of impurity center as short-range potential, then the correspondence of relaxation periods in the case of 2D and 3D systems does not depend on the type of potential. It equals:

$$\frac{\tau_{2D}(\varepsilon)}{\tau_{3D}(\varepsilon)}=\frac{2kw}{3\pi}, \qquad (8)$$

where k is the wave vector of electron in 3D systems: $k=\sqrt{\frac{2m^*}{\hbar^2}\varepsilon}$.

Based on this and the formula which we got earlier for $\tau_{3D}(\varepsilon)$ (4), we shall get:

$$\tau_{2D}(\varepsilon)=\frac{1}{6\pi^2}\frac{\varepsilon_0 m^2 w}{z^*\hbar^3 n_I}\left(\frac{a_0}{r_0}\right)^2\varepsilon\sim\varepsilon. \qquad (9)$$

So, electron's relaxation period depends on W depth of structure, also it depends on the radius of the area of influence of inner potential (1st part of (2) potential).

In the case of quasi-two-dimensional systems, electrons' mobility with non-degenerated electron system, based on [10] and [14] we can write:

$$\mu_{2D}(kT)=\frac{2e}{3m^*(k_0T)^2}\int_0^\infty \tau_{2D}(\varepsilon)\varepsilon e^{-\frac{\varepsilon}{k_0T}}d\varepsilon, \quad (10)$$

where k_0 is Boltzman constant. If we add (9) formula to this expression, we shall get:

$$\mu_{2D}(kT)=\frac{5e\varepsilon_0 m^2}{9\pi^2 m^* z^* \hbar^3 n_I} w\left(\frac{a_0}{r_0}\right)(k_0T)\sim(k_0T). \quad (11)$$

In [15] the mobility of 2D electron gas is calculated during dispersion on correlated distributed admixtures. According to these results, electrons' mobility in quasi-two-dimensional GaAs depends in direct proportion on temperature.

And for quasi-two-dimensional systems thermal electromotive force will be [11]:

$$\alpha_{2D}(T)=\frac{\pi^2}{3}\left(\frac{k_0}{e}\right)\left(\frac{k_0T}{E_f}\right)\left(1+E_f\frac{\partial\ln\tau_{2D}(\varepsilon)}{\partial\varepsilon}\right)_{\varepsilon=E_f}, \quad (12)$$

E_f is Fermi energy. So, based on (9) formula $\left(1+E_f\frac{\partial\ln\tau_{2D}(\varepsilon)}{\partial\varepsilon}\right)_{\varepsilon=E_f}=2$, so

$$\alpha_{2D}(T)=\frac{2\pi^2}{3}\left(\frac{k_0}{e}\right)\left(\frac{k_0T}{E_f}\right). \quad (13)$$

Our calculations' main criteria are Heisenberg's condition of using kinetic equation $\tau(\varepsilon)>>\frac{\hbar}{\varepsilon}$. This condition, based on (9) formula, lays down this condition:

$$w>>\frac{6\pi^2 z^*\hbar^4 n_I}{\varepsilon_0 m^2}\left(\frac{r_0}{a_0}\right)^2\frac{1}{(k_0T)^2}. \quad (14)$$

For example, if we consider non-degenerated, heavily doped with shallow impurities Ge and Si crystal, when $n_I\sim3\cdot10^{18}$cm^{-3}, at room temperature there still dominates dispersion on ionized admixtures [2]. This means that $w>>2\div3$ nm.

The results obtained in this paper, $\tau(\varepsilon)\sim\varepsilon$ and $\mu(k_0T)\sim(k_0T)$ are different from those obtained in other papers [10, 11], the individuality of impurity is also defined with the effective main quantum number n^* and with ionization energy of electron (first ionization energy).

ფიზიკა

ელექტრონების გაბნევა იონიზირებულ მინარევებზე კვაზიორგანზომილებიან ნახევარგამტარულ სისტემებში

ზ. გოგუა*, ა. გიგინეიშვილი*, გ. ილურიძე*, გ. რთველიაშვილი*, გ. კანტიძე*

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მოცემულ ნაშრომში ერთიანი მინარევული ცენტრის მოდელის გამოყენებით გათვლილია ელექტრონების რელაქსაციის დროის ენერგიაზე, ელექტრონების და ძვრადობის ტემპერატურაზე დამოკიდებულებები

კვაზიორგანზომილებიან, გადაუგვარებელ ნანოსტრუქტურებში. ნაჩვენებია, რომ ელექტრონის რელაქსაციის დრო და ძვრადობა დამოკიდებულია ნანოსტრუქტურის სისქეზე და ასევე დამოკიდებულია პირველი კოორდინაციული სფეროს რადიუსზე. დადგინდა, რომ ელექტრონების რელაქსაციის დროა $\tau(\varepsilon) \sim \varepsilon$, ძვრადობა კი $\mu(KT) \sim (\mathrm{KT})$, აგრეთვე გამოთვლილია თერმოელექტრომამოძრავებელი ძალაც.

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Received October, 2008