INFLUENCE OF THE IMPURITY FLUCTUATIONS ON THE ELECTRONIC AND TRANSPORT PROCESSES IN DOPING SUPERLATTICES

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INTRODUCTION

At high levels of the doping of a semiconductor the energy spectrum of current carriers changes. As a result of overlapping the impurity band with the nearest intrinsic band of the crystal, the tail of the density of states appears [1, 2]. Taking into account the tails is essential for interpretation of the electronic spectrum and transport processes in doping superlattices [3–7]. The state density tails also influence on the relation between the diffusion coefficient D and mobility μ [4–6] which belongs to one of the most important thermodynamical parameters of semiconductors.

The ratio D/μ attributes with the screening length, processes of diffusion and recombination, thermoelectric power, activity coefficient, photoconductivity, and time response of different optoelectronics semiconductor structures [8, 9]. In some specific physical conditions and systems, the diffusivity–mobility ratio D/μ exhibits anomalous behavior in dependence on the concentration of carriers and temperature. The class of such systems include heavily doped semiconductor materials with impurity bands and screened state density tails [8] as well as low-dimensional structures of quantum-well layers or quantum wires. Doping superlattices is another semiconductor system with anomalous character of the D/μ ratio [4–6].

In the paper, the influence of high doping on the energy spectrum and electron transport characteristics of *n-i-p-i* crystals is determined taking into account the Gaussian and exponential character of the fluctuated energy states. Influence of the impurity correlation on the D/μ ratio is examined in detail. Data of self-consistent calculations of the Schrödinger and Poisson's equations are presented for different temperatures of the crystal.

THEORY

The standard relation between the diffusion coefficient and mobility is given as

$$e\frac{D}{\mu} = n\frac{d\zeta_e}{dn}, \tag{1}$$

where n is the concentration of electrons, ζ_e is the chemical potential, i. e. the quasi-Fermi level for electrons F_e measured relatively to the conduction band bottom E_{c0}. In the case of the electric quantum limit, where the crystal temperature is sufficiently low and a main contribution in the electric conductivity is provided with the ground subband states, the expression for the two-dimensional concentration of electrons in the Gaussian approach has the form [5]

$$n = \frac{m_c \sigma_c}{2\pi\hbar^2}\left(x\mathrm{erfc}(-x) + \frac{1}{\sqrt{\pi}}\exp(-x^2)\right), \tag{2}$$

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Here, $x = (\zeta_e - E_{c00})/\sigma_c$, E_{c00} is the ground state energy. The characteristic parameter of the tail of the density of electron states σ_c is determined as [1, 2, 8]

$$\sigma_c = \frac{e^2}{\varepsilon}\sqrt{4\pi N_d L_c}, \tag{3}$$

where ε is the dielectric constant, N_d is the concentration of donors. The total screening length L_c with taking into account the impurity correlation in n-layers of the structure equals [7]

$$L_c = L_d\left(1+\frac{L_d^2}{L_n^2}\right)^{-1/2}, \tag{4}$$

where L_n and L_d are the screening lengths related to electrons and donor impurities. The values of L_n and L_d cab be evaluated according to the expressions

$$L_n = \left(\frac{4\pi e^2}{\varepsilon\, d_n}\left(\frac{dn}{d\zeta_e}\right)\right)^{-1/2}, \qquad L_d = \left(\frac{4\pi e^2 N_d}{\varepsilon k T_0}\right)^{-1/2}. \tag{5}$$

Here, d_n is the thickness of n-layers, T_0 is the "freezing" temperature. Using Eqs. (1) and (2), one obtains the generalized D/μ ratio [5], i. e.,

$$e\frac{D}{\mu} = \sigma_c\left(\eta_c + \frac{e^{-\eta_c^2}}{\sqrt{\pi}\,\mathrm{erfc}(-\eta_c)}\right), \tag{6}$$

where $\eta_c = (F_e - E_{c0} - E_{c00})/\sigma_c \equiv x$ is the parametric quantity.

The generalized expression for the diffusivity–mobility ratio in the case of exponential state density tails has the form

$$e\frac{D}{\mu} = E_0\left(1+e^{-\eta}\right)\ln\left(1+e^{\eta}\right), \tag{7}$$

where $E_0 = \sigma_c/a_u$, $\eta = a_u\eta_c$, $a_u = 2.565$. The comparison of the Gaussian and exponential generalized calculations is shown in Fig. 1(*a*).

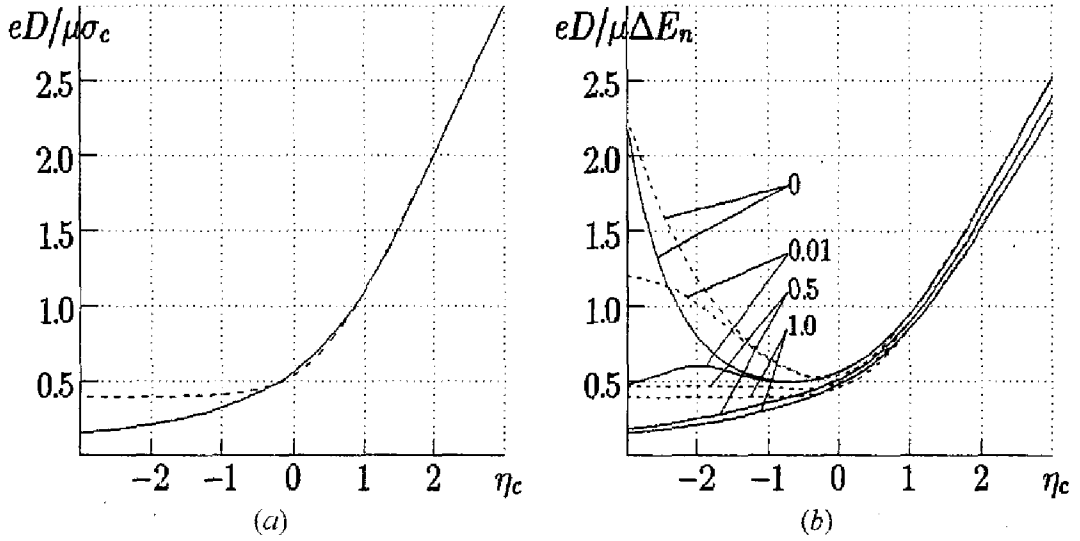

Figure 1 – (*a*) The generalized diffusivity–mobility ratio D/μ calculated with taking into account the Gaussian (solid curves) and exponential (dashed curves) state density tails and (*b*) values of D/μ at different impurity correlation coefficients C (values at the curves). $d_n/2a_3 = 1$.

Including the impurity correlation based on Eqs. (3)–(6) gives the expression for the D/μ ratio in the form

$$e\frac{D}{\mu}=\frac{\sigma_{c0}}{(\mathrm{erfc}(-\eta_c)+C)^{1/4}}\left(\eta_c+\frac{e^{-\eta_c^2}}{\sqrt{\pi}\,\mathrm{erfc}(-\eta_c)}\right), \tag{8}$$

where $C=L^2_{c,\eta_c=0}/L_d^2$ is the impurity correlation coefficient. The value of the σ_{c0} is equal to

$$\sigma_{c0}=\left(\frac{d}{2a_3}\right)^{1/4}\Delta E_n=\left(\frac{d}{2a_3}\right)^{1/4}\frac{e^2}{\varepsilon}\sqrt{4\pi N_d a_3}\,, \tag{9}$$

where a_3 is the effective Bohr radius. At $\eta_c \gg 1$, the relation $eD/\mu \approx \sigma_{c0}(2+C)^{-1/4}\eta_c$. When $\eta_c=0$, the value $eD/\mu=\sigma_{c0}/\sqrt{\pi}(1+C)^{1/4}$. If $\eta_c \ll 1$, then the D/μ ratio decreases inversely proportionally $|\eta_c|$ and equals $\sigma_{c0}/2C^{1/4}|\eta_c|$. As it is shown in Fig. 1(*b*), maximum and minimum values of D/μ versus η_c with increasing the coefficient C approach to each other, and at $C>0.057$ the extremums disappear.

In the similar way, the expression for the D/μ ratio is obtained in the case of the exponential state density tails and impurity correlation, i. e.,

$$e\frac{D}{\mu}=E_{00}\left(\frac{2}{1+e^{-\eta}}+C\right)^{-1/4}\left(1+e^{-\eta}\right)\ln\left(1+e^{\eta}\right), \tag{10}$$

where $E_{00}=\sigma_{c0}/a_u$. For large positive values of η, curves of the D/μ ratio at the Gaussian and exponential state density tails coincide. At $\eta=0$, we find $eD/\mu=2\sigma_{c0}\ln 2/a_u(1+C)^{1/4}$ that is slightly smaller as compared the Gaussian approach. In the deep states of the tail $\eta \ll -1$, the D/μ ratio for the exponential model has the fixed value of $E_{00}/C^{1/4}$. With increasing the impurity correlation coefficient C the minimum of D/μ shifts to smaller values of η_c and then disappears. At $C=0$, where no "background" impurity screening, Eqs. (8) and (10) are simplified.

In doping superlattices, electron and hole quantum wells are spatially separated and, as a rule, the screening length is smaller compared with the superlattice period: Therefore, random fluctuations of the impurity concentrations manifest themselves independently in *n*- and *p*-regions [4–6]. Data of self-consistent calculations of the diffusivity–mobility ratio for electrons D_n/μ_n and holes D_p/μ_p at different temperatures are presented in Fig. 2.

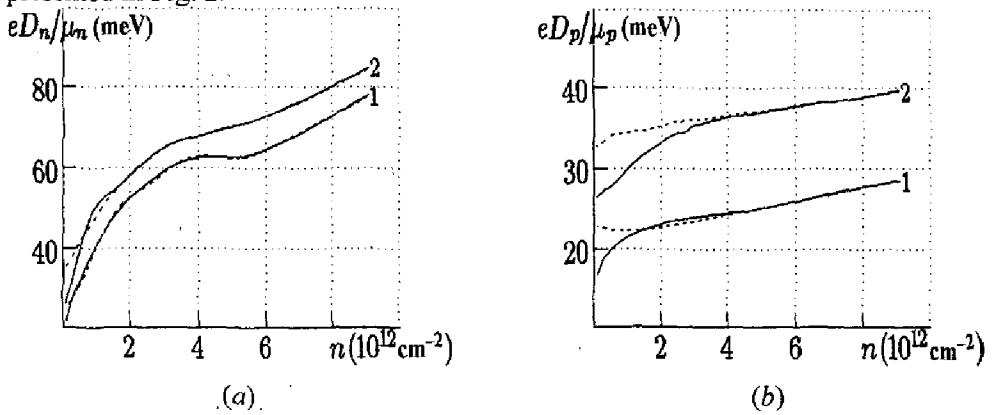

Figure 2 – The diffusivity–mobility ratio D/μ for (*a*) electrons and (*b*) holes versus the surface electron concentration n calculated with taking into account the Gaussian (solid curves) and exponential (dashed curves) state density tails for different temperatures (1) $T=4.2$ and (2) 300 K, $N_a=N_d=2\times10^{18}$ cm^{-3}, $d_p=d_n=7$ nm, $d_i=0$.

As it is seen, at low concentrations of current carriers the D/μ ratio calculated for the exponential state density tails approaches the limit $E_{00}/C^{1/4}$. Results for the Gaussian model of the density of states show that at the decrease of the carrier concentration the diffusivity–mobility ratio tends to the classical value kT/e.

CONCLUSION

The relation between the diffusion coefficient and mobility of current carriers at filling the electron and hole subbands exhibits an anomalous character in dependence on the carrier concentrations and temperature. This behavior of the diffusivity–mobility ratio occurs in the electric quantum limit and at room temperature as well. Described features give additional possibilities to study design parameters and the energy spectrum of doping superlattices and to understand the role of the fluctuating impurity potential. Different electronic processes in *n-i-p-i* crystals, including the giant ambipolar diffusion, are connected with the examined screening and impurity correlation effects.

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