Abnormal Character of the Diffusivity-mobility Ratio in Doping Superlattices

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The influence of high level of doping in type n-i-p-i crystal structures on electron and hole state distributions is examined. Abnormal behaviour in the diffusivity- mobility ratio due to shortening of the density state tails under excitation of doping Superlattices is described.

Key words: crystal structures, doping, diffusion

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1 Introduction

The relation between diffusion coefficient D and mobility μ of current carriers is one of the most important thermodynamical parameters of semiconductors [1]. The ratio D/μ, attributes with the screening length, processes of diffusion and recombination, thermoelectric power, activity coefficient, photoconductivity, and time response of different optoelectronic semiconductor structures [2]. In some specific physical conditions and systems the diffusivity-mobility ratio exhibits abnormal behaviour in dependence on the concentration of carriers and temperature. Such systems include heavily doped semiconductor materials with impurity state bands [3] and screened density states tails [4] as well as low-dimensional structures of quantum- well layer or quantum wire types [5], [6]. Doping Superlattices is one more semiconductor system with abnormal character of D/μ ratio.

Doping Superlattices, or n - i - p - i crystals, consist of n- and p-type semiconductor layers separated by the intrinsic layers. Electrostatic potential profile and electron and hole energy state spectra in doping Superlattices depend on dopant concentrations and layer thicknesses as well as level of excitation [7], [8]. In this work, fluctuations of impurity concentrations in doped regions of n - i - p - i crystals have been taking into account and the relation between diffusion coefficient and mobility of quantum-confined carriers has been considered.

2 Density of states in doping superlattices

At high levels of doping of a semiconductor the energy spectrum of current carriers changes [9]. Because of overlapping of the impurity band with the nearest intrinsic band of a crystal, the tail of the density of states appears. Account of the tails is important for interpretation of electric and optical phenomena in doped semiconductors. In particular, in spectra of absorption, gain, and luminescence of the structures based on doping superlattices a significant long-wavelength tail is observed [10]. Taking into consideration the fluctuations of the impurity concentrations gives an opportunity to explain the experimental data.

To determine the density of states in doping superlattices, the method developed for heavily doped bulk semiconductors will be used [4], [11]. When taken into account random (Gaussian statistics) fluctuations of doping impurity concentrations, the distribution of the density of states versus energy E in the conduction band is represented in the form [12]

$$\rho_c(E) = \frac{m_c}{2\pi\hbar^2 N_p} \times \sum_{n,\nu} erfc\left(\frac{E_{c0} + E_{cn\nu} - E}{\sigma_c}\right), \quad (1)$$

where m_c is the effective mass of electrons, N_p is the number of superlattice periods, E_{c0} is the energy of conduction band bottom, $E_{cn\nu}$ is the quantization electron level energy, n and ν are quantum numbers of electron subbands and minisubbands. The total number of states in the minisubbands is equal to N_p but some states are degenerated. The tail spreading of the density of electron states is determined by the characteristic parameter σ_c. Similar expression is obtained for the distribution of the density of holes states $\rho_\upsilon(E)$ with the characteristic tail parameter σ_υ.

In doping superlattices, n- and p-layers are spatially separated and, therefore, the random distributions of impurities in different doped regions are independent. The tail parameters are determined by average values of donor and acceptor concentrations N_d and N_a and by screening lengths L_e and L_h in n- and p-regions, respectively. The expressions for the tail parameters have the form [4], [9], [11]

$$\sigma_c = \frac{e^2}{\epsilon}\sqrt{4\pi N_d L_e}, \quad \sigma_\upsilon = \frac{e^2}{\epsilon}\sqrt{4\pi N_a L_h}, \qquad (2)$$

where ϵ is the dielectric constant of semiconductor. The screening lengths in n- and p-regions of the superlattice can be evaluated in two-dimensional electron gas limit as follows [13]

$$\frac{1}{L_e} = \frac{2\pi e^2}{\epsilon}\cdot\frac{dn}{d\zeta_e}, \quad \frac{1}{L_h} = \frac{2\pi e^2}{\epsilon}\cdot\frac{dp}{d\zeta_h}. \qquad (3)$$

Here n and p are two-dimensional concentrations of electrons and holes, $\zeta_e = F_e - E_{c0}$ and $\zeta_h = E_{\upsilon 0} - F_h$ are chemical potentials, F_e and F_h are quasi-Fermi levels for electrons and holes, respectively. The energy $E_{\upsilon 0}$ is related to the top of the valence band and hence the effective band gap of the superlattice $E_g' = E_{c0} - E_{\upsilon 0}$. It depends on the depth of the potential relief $2\Delta V$ as $E_g' = E_g - 2\Delta V$, where E_g is the band gap of the host semiconductor. The shape and depth of the potential relief in doping superlattices is connected with the design parameters such as impurity concentrations N_d and N_a and thicknesses of n-, p-, and i-layers d_n, d_p, and d_j. Increasing the nonequilibrium carrier concentration results in the transformation of the superlattice energy band structure [8]. Therewith, the condition $p = n + N_a d_p - N_d d_n$ is fulfilled.

In the framework model, the self-consistent solution of the Schrodinger and Poisson's equations

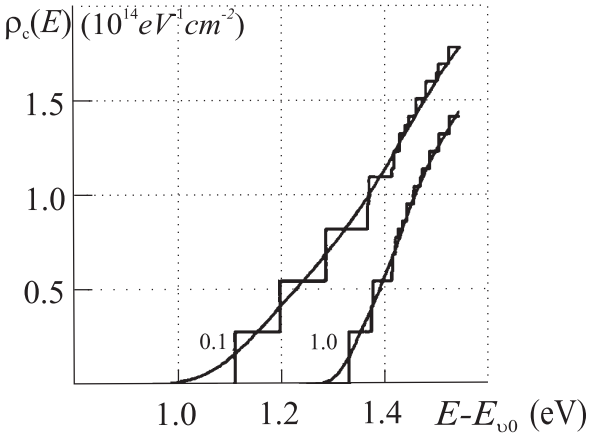

FIG. 1. Distributions of the density of states in the conduction band $\rho_c(E)$ at different pump factors r (numbers at the curves) without (step curves) and with taking into account the density state tails (smooth curves). $N_a = 10^{19}cm^{-3}$, $N_d = 6\times10^{18}cm^{-3}$, $d_n = d_p = 15nm$, $d_i = 0$, $N_p = 6$, $T = 300K$. $\sigma_c = 93meV$, $E_g' = 1.08eV$ *at* $r = 0.1$ and $\sigma_c = 37meV$, $E_g' = 1.32eV$ *at* $r = 1.0$.

was numerically obtained [12]. Calculated distributions of the density of states for electrons in GaAs p-type doping superlattice under excitation are shown in Fig. 1. As seen, fluctuations of impurity concentrations smooth the ideal step-like state distribution. Increasing the excitation pump leads to the decrease of the screening lengths and, accordingly, shortening the tails of the density of states. The level of excitation is determined by the pump factor $r = n/N_d d_n$. At increasing r the modulation depth of the potential profile $2\Delta V$ decreases and the value of E_g' approaches to E_g.

3 Peculiarities of the diffusivity-mobility ratio

Deformations of energy spectrum in quantum wells of doping superlattices, because of high levels of doping with donors and acceptors, are reflected on D/mu ratio. Standard relation between the diffusion coefficient and mobility for electrons in n-

regions and for holes in p-regions of the superlattice has the form

$$\frac{D_n}{\mu_n} = \frac{n}{e} \cdot \frac{d\zeta_e}{d_n}, \quad \frac{D_p}{\mu_p} = \frac{p}{e} \cdot \frac{d\zeta_h}{d_p}. \tag{4}$$

Here the subscripts n and p correspond to n- and p-regions,respectively.

Two-dimensional concentration of carriers, e.g., of electrons, when taking into account the tail of the density of states, is determined by the expression

$$n = \frac{N_{c1}}{N_p} \sum_{n,\nu} \frac{1}{2} \left[x_c erfc(-\alpha_c x_c) + \left(\frac{1}{\sqrt{\pi}\alpha_c} + \right. \right. \\ \left. \left. + F\left(\alpha_c, q_c\right) \right) e^{-\alpha_c^2 x_c^2} \right], \tag{5}$$

where $N_{c1} = m_c kT/\pi\hbar^2$ is the sheet effective follows density of states in the conduction band per period of the superlattice, T is the temperature, $x_c = (\zeta_e - E_{cn\nu})/kT$, $\alpha_c = kT/\sigma_c$, $q_c = 2\alpha_c^2 x_c$.

The function $F(\alpha_c, q_c)$ is represented by the sum

$$F(\alpha_c, q_c) = \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k} \left[\exp\left(\frac{k+q_c}{2\alpha_c}\right)^2 \right. \\ \left. \times \mathrm{erfc}\left(\frac{k+q_c}{2\alpha_c}\right) + \exp\left(\frac{k-q_c}{2\alpha_c}\right)^2 \mathrm{erfc}\left(\frac{k-q_c}{2\alpha_c}\right) \right]. \tag{6}$$

It has minimum at $q_c = 0$ and is proportional to q_c^2. E.g., the function $F(\alpha_c, q_c)$ at α_c=1 can be approximated by $F(\alpha_c, g_c) == 0.93 + 0.16 q_c^2$.

When Eq. (5) is substituted into Eq. (4), the following relation between the diffusion coefficient and mobility of electrons been in n-regions of the n - i-p - i crystal is fulfilled

$$e\frac{D_n}{\mu_n} = kT \frac{\sum_{n,\nu} \left[x_c erfc(-\alpha_c x_c) + \left(\frac{1}{\sqrt{\pi}\alpha_c} + F(\alpha_c, q_c) \right) e^{-\alpha_c^2 x_c^2} \right]}{\sum_{n,\nu} [erfc(-\alpha_c x_c) + R(\alpha_c, q_c) e^{-\alpha_c^2 x_c^2}]} \tag{7}$$

Here, the sum

$$R(\alpha_c, q_c) = \sum_{k=1}^{\infty} (-1)^{k+1} \left[\exp\left(\frac{k+q_c}{2\alpha_c}\right)^2 erfc\left(\frac{k+q_c}{2\alpha_c}\right) - \exp\left(\frac{k-q_c}{2\alpha_c}\right)^2 erfc\left(\frac{k-q_c}{2\alpha_c}\right) \right] \tag{8}$$

equals 0 at $q_c = 0$. When $\alpha_c = 1$, the function $R(\alpha_c, q_c)$ in the region near $q_c = 0$ behaves approximately as $R(l, q_c) = -0.29 q_c$. Analytical and numerical methods of calculations of the functions $F(\alpha_c, q_c)$ and $R(\alpha_c, q_c)$ have been described earlier [12].

In quantum limit, where the crystal temperature is sufficiently low and the main contribution in the electrical conductivity is due to the ground subband, D/μ ratio for electrons behaves according to Eq. (7) as

$$e\frac{D_n}{\mu_n} = \zeta_e - E_{c00} + \frac{\sigma_c}{\sqrt{\pi}} \cdot \frac{\exp\left(-\left(\frac{\zeta_e - E_{c00}}{\sigma_c}\right)^2\right)}{erfc\left(-\frac{\zeta_e - E - c00}{\sigma_c}\right)} \tag{7}$$

Here, the tail parameter σ_c depends on chemical potential ζ_e.

When quasi-Fermi level $F_e$crosses the ground subband state E_{c00} the value of eD_n/μ_n reaches

$\sigma_c/\sqrt{\pi}$. If tail states are neglected, the D_n/μ_n ratio follows proportionally to ζ_e that corresponds to the case of quantum-well layers [5], [6]. By analogy with Eq. (7) the expression which connects the ratio D_p/μ_p for holes with the tail parameter σ_υ and screening length L_h in p-regions of the superlattice is apparently written. Taking into account heavy and light holes, one has

$$e\frac{D_p}{\mu_p} = kT\frac{\sum\limits_i m_{vit}\sum\limits_{m,\nu}\left[x_\upsilon erfc(-\alpha_\upsilon x_\upsilon) + \left(\frac{1}{\sqrt{\pi}\alpha_\upsilon} + F(\alpha_\upsilon, q_\upsilon)\right)e^{-\alpha_\upsilon^2 x_\upsilon^2}\right]}{\sum\limits_i m_{vit}\sum\limits_{m,\nu}[erfc(-\alpha_\upsilon x_\upsilon) + R(\alpha_\upsilon, q_\upsilon)e^{-\alpha_\upsilon^2 x_\upsilon^2}]} \qquad (10)$$

where $x_\upsilon = (\zeta_h - E_{vim\nu}/kT, a_\upsilon = kT/\sigma_\upsilon, q_\upsilon = 2\alpha_\upsilon^2 xv, E_{vim\nu}$ is the quantization level energy for heavy ($i = h$) and light ($i = l$) holes, m and ν are quantum numbers of hole subbands and minisubbands. The functions $F(\alpha_\upsilon, q_\upsilon)$ and $R(\alpha_\upsilon, q_\upsilon)$ are similar to the sums given by Eqs, (6) and (8). In general case, the transverse effective masses for heavy and light holes m_{vit} differ from the effective masses m_{vi} along the dimensional quantization axis. When calculating σ, L, and D/μ for the GaAs doping superlattices, the band parameters as for the GaAs quantum-well laser structures have been used, in particular, $m_c = 0.066m_e, m_{vh} = 0.34m_e, m_{vl} = 0.093m_e, m_{vht} = 0.12m_e$, and $m_{vlt} = 0.22m_e$ [14]. The results of the calculations are shown in Figs. 2 and 3. For p-type doping superlattice, the screening length and tail parameter for electrons are higher than for holes . At increasing the pump factor $r = n/N_d d_n$ the screening lengths decrease and the tails of the density of states become shorter.

As seen from Fig. 3, the D/μ, ratio exceeds the classical value kT/e. The described abnormal change of the D/μ, ratio is conditioned by shortening the tails due to the effect of screening by nonequilibrium current carriers. For compensated superlattices, decrease of D/μ, at increasing r occurs for both electrons and holes (Fig. 3a). In p-type superlattices, abnormal behaviour in D/μ takes place for electrons only (Fig. 3b). In this case, the density tails in n-regions are shorten the most strongly. The values of L_e and L_h are found to be smaller as compared with the superlattice period. Therefore, the screening of the fluctuated impurity charge potential in doping superlattices is actually accomplished by current carriers only of a certain type, i.e., by electrons in n-regions and by holes in p-regions.

As a result, in p-type superlattice, the tail of the density of states is effectively reduced in n- regions under excitation, but in p-regions the energy spectrum does not practically change. The value of eD_n/μ_n for electrons decreases, in particular, at room temperature from 74 to 52 meV at the initial stage of superlattice excitation (Fig. 3b). This abnormal change of D/μ, ratio is much greater as compared with the bulk GaAs crystal [4] or ordinary quantum-well structures [5]. Established features of the relation between D and μ, have to be taken into account at the analysis of characteristics of light emitting structures and photosensitive elements based on doping superlattices.

4 Conclusion

The fluctuated impurity change potential, because of random distributions of dopants in different doped regions, smoothes the step-like distributions of the density of states for electrons and holes in doping superlattices. Increasing the nonequilibrium current carriers under excitation results in decreasing the screening lengths in n- and p-regions and shortening the tails of the density of states. It reflects on the diffusivity-mobility ratio that exhibits the abnormal behaviour, i.e., the D/μ, ratio decreases at increasing excitation power.

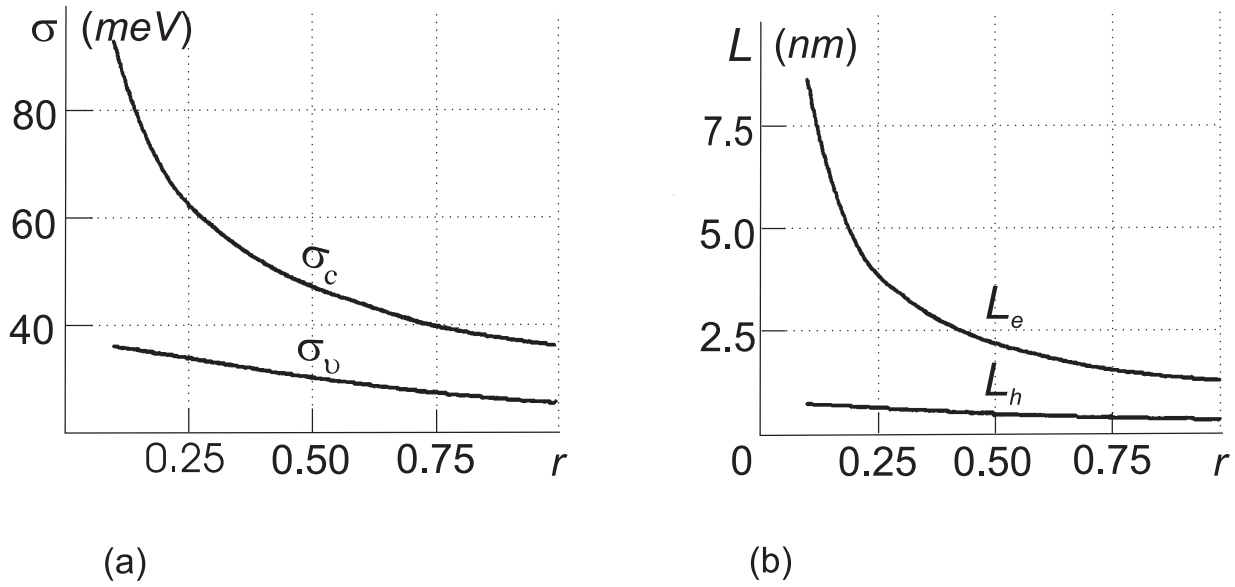

FIG.2. (a) Parameters of density state tails $\sigma = \sigma_c$ or σ_v and (b) screening lengths L = L_e or L_h, in n- or p-regions, respectively, versus the pump factor r. $N_a = 1019cm^{-3}, N_d = 6x10^{-18}cm^{-3}, d_n = d_p = 15nm, d_i = 0, T = 300K$.

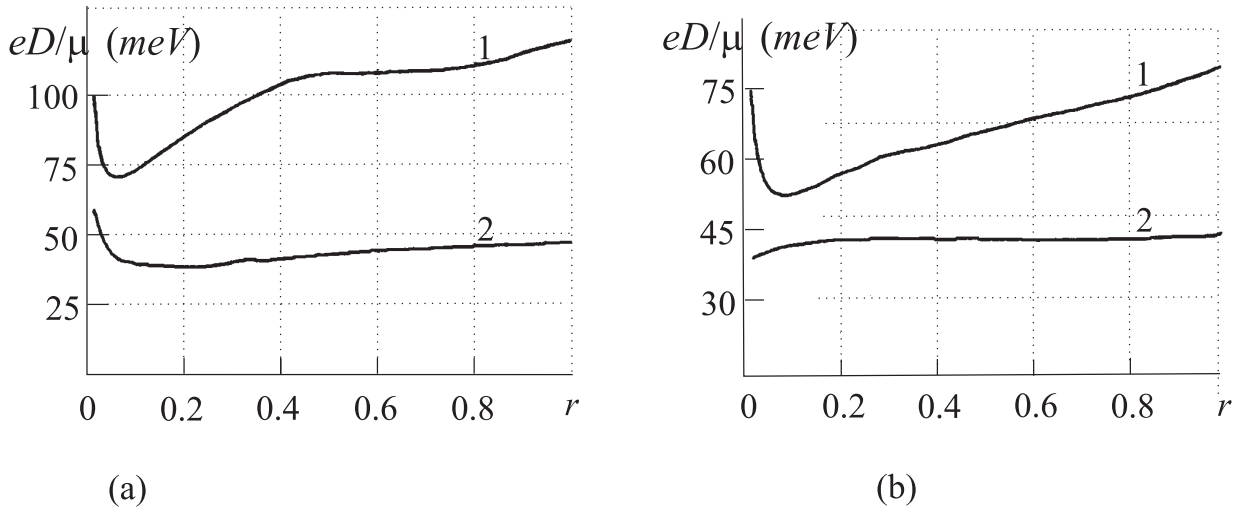

FIG.3. Diffusivity-mobility ratio for (1) electrons and (2) holes versus the pump factor r. (a) $N_a = N_d = 10^{19}cm^{-3}$ $(b) N_a = 10^{19}cm^{-3}, N_d = 5x10^{18}cm^{-3}, d_p = d_n = 15nm, d_i = 0, T = 300K$.

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