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Carrier Transport and Screening in n–i–p–i Crystals

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The variation of the energy spectrum of n–i–p–i crystals under excitation was examined and the influence of the reduction of the screening length on the ratio between the coefficient of diffusion and the mobility of the current carriers was established. It is shown that the filling of subband states by carriers results in an anomalous behaviour of the diffusivity–mobility ratio. The effect occurs in the electric quantum limit and at room temperature as well.

1. Introduction

Doping superlattices, or n–i–p–i crystals, possess a tunable energy spectrum under excitation. Accordingly, both electrical and optical characteristics change [1]. High level of doping in n- and p-type regions and fluctuations of impurity concentrations in n–i–p–i crystals modify the step-like distribution of the density of states. This influence is controlled by screening which varies with the filling of subband states by current carriers. In this paper, the energy spectrum of doping superlattices is analyzed, effects of screening of the electrostatic potential are taken into account, and peculiarities of the relation between the coefficient of diffusion and the mobility of quantum-confined carriers are considered.

2. Tails of the Density of States

At high levels of doping of a semiconductor crystal the energy spectrum of current carriers changes [2]. Because of overlapping of the impurity band with the nearest intrinsic band of the crystal, a tail of the density of states appears. Taking account of the tails is important for the interpretation of electrical and optical phenomena in doped semiconductors.

To determine the density of states in doped superlattices, a method developed for heavily doped bulk semiconductors will be used [3, 4]. When random fluctuations of doping impurity concentrations, which follow the Gauss statistics, are taken into account, the distribution of the density of states versus the energy E in the conduction band is represented in the form [5]

$$\varrho_c(E) = \frac{m_c}{2\pi\hbar^2 N_p} \sum_n \sum_\nu \operatorname{erfc}\left(\frac{E_{c0} + E_{cn\nu} - E}{\sigma_c}\right). \qquad (1)$$

Here, m_c is the effective mass of electrons, N_p is the number of superlattice periods, E_{c0} is the energy of the bottom of the conduction band, $E_{cn\nu}$ is the quantization level en-

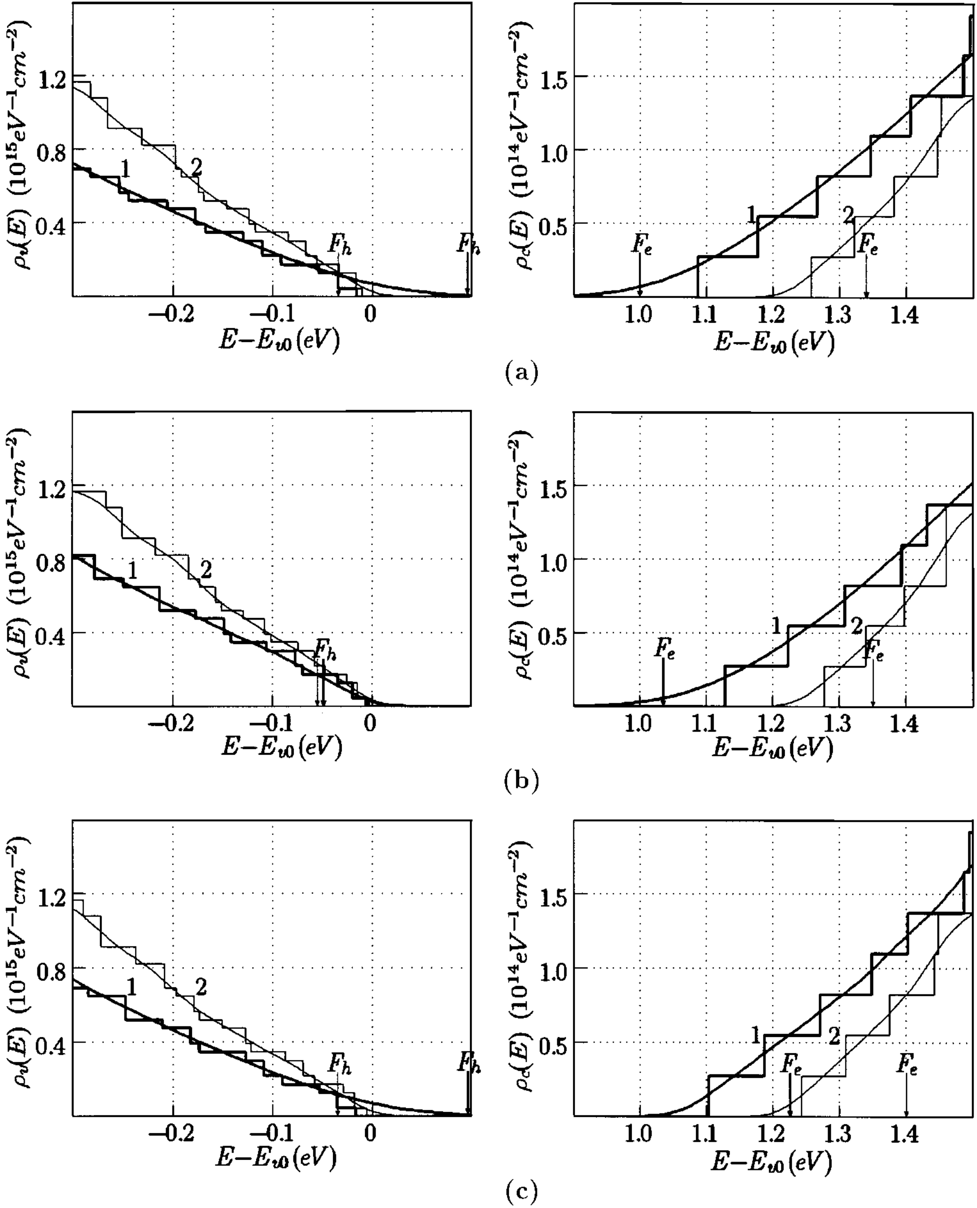


Fig. 1. Distributions of the density of states in the conduction band $\varrho_c(E)$ and valence band $\varrho_v(E)$ at different concentrations of current carriers without (step curves) and with taking into account the density of state tails (smooth curves). a) A compensated superlattice, $N_a = N_d = 5\times10^{18}$ cm^{-3}, (1) $r = 0.04$, $\sigma_c = 140$ meV, $\sigma_v = 112$ meV, $E'_g = 1.03$ eV, (2) $r = 0.4$, $\sigma_c = 48$ meV, $\sigma_v = 29$ meV, $E'_g = 1.22$ eV; b) p-type superlattice, $N_a = 8\times10^{18}$ cm^{-3}, $N_d = 5\times10^{18}$ cm^{-3}, (1) $r = 0.04$, $\sigma_c = 140$ meV, $\sigma_v = 34$ meV, $E'_g = 1.08$ eV, (2) $r = 0.4$, $\sigma_c = 48$ meV, $\sigma_v = 28$ meV, $E'_g = 1.24$ eV; c) n-type superlattice, $N_a = 5\times10^{18}$ cm^{-3}, $N_d = 8\times10^{18}$ cm^{-3}, (1) $r = 0.4$, $\sigma_c = 58$ meV, $\sigma_v = 112$ meV, $E'_g = 1.06$ eV, (2) $r = 0.62$, $\sigma_c = 48$ meV, $\sigma_v = 30$ meV, $E'_g = 1.21$ eV

ergy for electrons, n and ν are the quantum numbers of electron subbands and minisubbands, respectively. The total number of states in a minisubband 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. A similar expression is obtained for the distribution of the density of holes states $\varrho_v(E)$ with the characteristic tail parameter σ_v.

Within the framework of the model, the self-consistent solution of the Schrödinger and Poisson's equations was numerically produced [5]. The calculated distributions of the density of states of electrons and holes in the GaAs doping superlattices under excitation are shown in Fig. 1. For simplicity, the calculations were performed at $N_p = 1$. The temperature T was supposed to be equal to 4.2 K and anisotropy of effective masses of heavy and light holes was taken into account. The values of quantization level energies depend on the doping superlattice design parameters, such as the concentrations of donors N_d and acceptors N_a and the thicknesses of n-layers d_n, p-layers d_p, and i-layers d_i. In Fig. 1, the energy E is given relative to the top of the valence band E_{v0}, $d_n = d_p = 15$ nm, $d_i = 0$. The positions of the quasi-Fermi level for electrons F_e and for holes F_h are indicated. The shape of the potential profile in doping superlattices is determined by the current carrier concentrations, and, therefore, the energy spectrum depends on the level of excitation of the crystal.

As seen from Fig. 1, fluctuations of impurity concentrations smooth the ideal step-like state distribution. Increasing the excitation level, i.e. the concentrations of nonequilibrium current carriers, leads to a decrease of the screening lengths and, accordingly, a reduction of the tails of the density of states. It is convenient to express the level of excitation by the pump factor $r = n/N_d d_n$, where n is the two-dimensional concentration of electrons in n-regions. At increasing r the modulation depth of the potential profile decreases and the value $E'_g = E_{c0} - E_{v0}$ approaches the band gap of the host semiconductor E_g.

Mention that the Gauss statistics for fluctuations of impurity concentrations and the linear screening assumptions approach the least for the description of deep levels at the tails of the density of states, though the limitations for impurity and carrier concentrations prove to be very relative [2 to 4]. Therefore, the developed self-consistent model is adequately applicable for n–i–p–i crystals at a sufficiently marked level of excitation, i.e., when r is approximately above 0.04. A comparison of different models taking into consideration disorder effects on luminescence spectra in n–i–p–i crystals with δ-doped layers is carried out in [6].

3. Electric Quantum Limit

In doping superlattices, electron and hole quantum wells are spatially separated and, as follows from calculations, the screening length is small in comparison with the superlattice period. Therefore, random fluctuations of dopant concentrations manifest themselves independently in n- and p-regions. In particular, the tail parameter σ_c is determined as [2 to 4]

$$\sigma_c = \frac{e^2}{\epsilon} \sqrt{4\pi N_d L_e}\,, \tag{2}$$

where ϵ is the static dielectric constant of the semiconductor, L_e is the screening length in n-regions of the n–i–p–i crystal. The value of L_e can be evaluated in the two-dimen-

sional electron gas limit from the expression [7]

$$L_e = \frac{\epsilon}{2\pi e^2} \frac{d\zeta_e}{dn} . \tag{3}$$

Here, 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}. The three-dimensional screening length in the linearized Thomas-Fermi approximation taking into account the effect of impurity concentration fluctuations on the luminescence spectra in doping superlattices is used in [8].

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, one has

$$n = \frac{m_c \sigma_c}{2\pi\hbar^2} \left(x \operatorname{erfc}(-x) + \frac{1}{\sqrt{\pi}} \exp(-x^2) \right) , \tag{4}$$

where $x = (\zeta_e - E_{c00})/\sigma_c$. If the tail of the density of states is negligible, equation (4) transforms to the known expression for the degenerate electron gas in quantum-well layers when only one subband is taken into account. Using equation (4) and the standard relation between the coefficient of diffusion D and mobility μ of carriers one obtains the expression

$$e \frac{D}{\mu} = \sigma_c \left(x + \frac{\exp(-x^2)}{\sqrt{\pi} \operatorname{erfc}(-x)} \right) . \tag{5}$$

Here, the tail parameter σ_c depends on the chemical potential ζ_e. When the quasi-Fermi level F_e crosses the subband ground state E_{c00}, i.e. $x = 0$, the ratio eD/μ makes up the value of $\sigma_c/\sqrt{\pi}$ (Fig. 2). For large positive quantities of x the D/μ ratio follows proportionally ζ_e. Such dependence, obviously, corresponds to the case of quantum-well layers [9, 10].

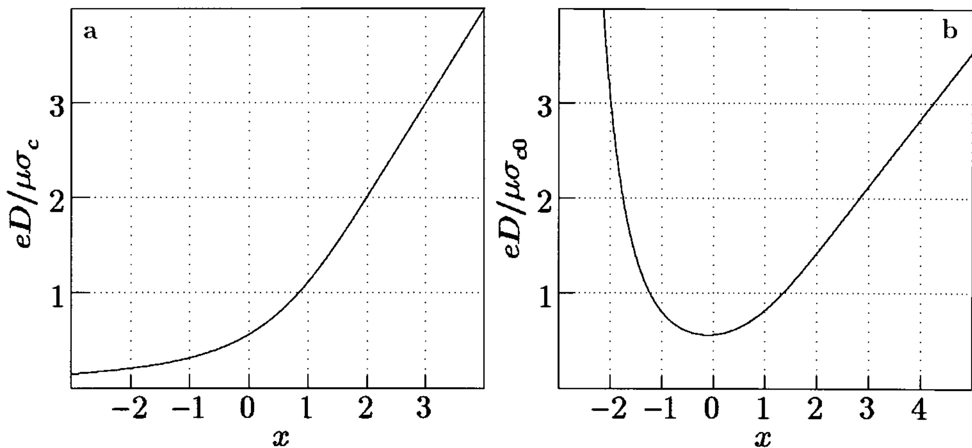


Fig. 2. The D/μ ratio normalized to a) σ_c or b) σ_{c0} in dependence on the value $x = (\zeta_e - E_{c00})/\sigma_c$

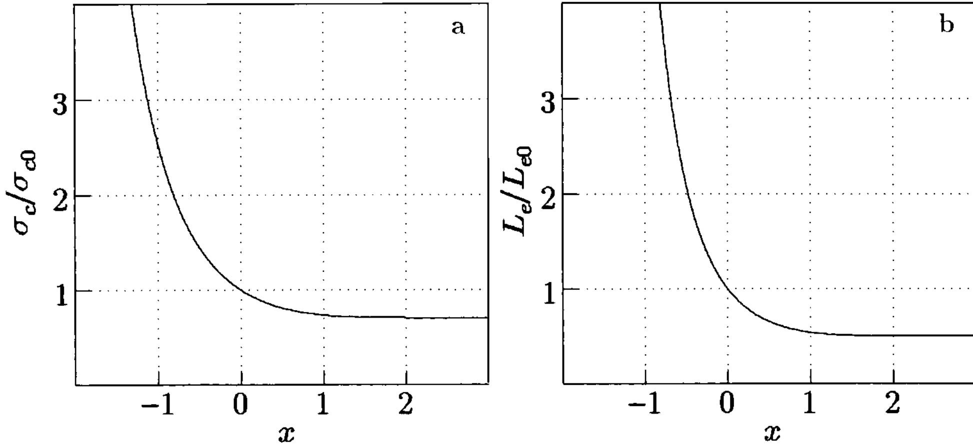


Fig. 3. a) The density of state tail parameter σ_c and b) screening length L_e versus the value x

Because of shortening the tails of the density of states due to screening by current carriers, the D/μ ratio exhibits an anomalous behaviour. It has a minimum versus the carrier concentration. A self-consistent consideration gives

$$e\,\frac{D}{\mu} = \sigma_{c0}\,\frac{\sqrt{\pi}\,x\,\mathrm{erfc}\,(-x) + \exp\,(-x^2)}{\sqrt{\pi}\,\mathrm{erfc}^{3/2}\,(-x)}\,. \tag{6}$$

Therewith, the tail parameter σ_c and screening length L_e change as follows:

$$\sigma_c = \frac{\sigma_{c0}}{\mathrm{erfc}^{1/2}\,(-x)}\,, \tag{7}$$

$$L_e = \frac{L_{e0}}{\mathrm{erfc}\,(-x)}\,. \tag{8}$$

The values $\sigma_{c0} = 2e\hbar\sqrt{\pi N_d/\epsilon m_c}$ and $L_{e0} = \epsilon\hbar^2/e^2 m_c$ correspond to the point $x = 0$. The minimum value of the D/μ ratio is reached at $x = -0.1$, i.e., practically where the quasi-Fermi level approaches the ground state of a subband. As the screening length L_e approaches the effective two-dimensional Bohr radius $L_{e0}/2$ at the filling of subband states by carriers, the shortest tail of the density of states is determined by the parameter $\sigma_c = \sigma_{c0}/\sqrt{2}$ (Fig. 3). It is interesting to mention that the quantity σ_{c0} equals the energy separation of quantization levels in parabolic parts of the potential relief.

4. Discussion and Results for GaAs n–i–p–i Crystals

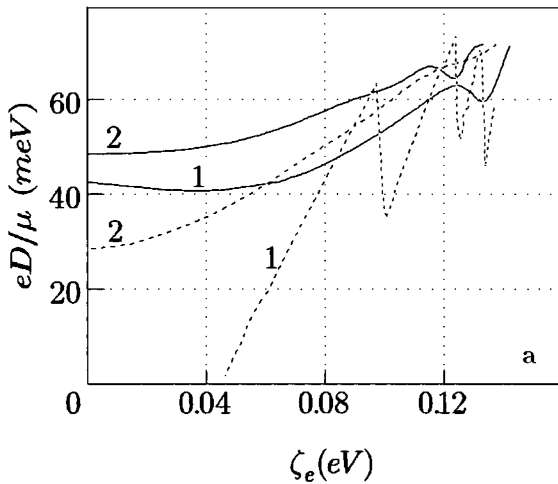
An anomalous behaviour of the D/μ ratio in doped semiconductors was predicted at first in [11] and is related to the transition from the impurity conductivity to the intrinsic band transport. The anomalous change of the D/μ ratio in n–i–p–i crystals results from the shortening of the tails of the density of states due to the effect of screening by current carriers. A similar phenomenon in bulk doped crystals was described earlier in

[4]. Another type of anomalous behaviour in the D/μ ratio takes place in quantum-well systems and is connected with carriers filling the states in high-lying subbands [10]. This effect is more clearly pronounced at low temperatures.

In n–i–p–i crystals, effects of filling the subband states and shortening the tails of the density of states act in common. But fluctuations of dopant concentrations smooth the dependencies of the D/μ ratio on the chemical potential or carrier concentrations. Therefore, the anomalous effect of filling the subband states can be pronounced only at a high level of superlattice excitation when the density state tails are greatly reduced.

For compensated doping superlattices ($N_a d_p = N_d d_n$), the anomalous decrease of D/μ at increasing carrier concentrations occurs for both electrons in n-regions and holes in p-regions. In p-type superlattices ($N_a d_p > N_d d_n$), the density of state tails decrease most strongly in the conduction band. As a result, the value of D/μ exhibits an anomalous behaviour to begin with electrons in n-regions. In n-type superlattices ($N_a d_p < N_d d_n$), an anomalous change of D/μ occurs with holes in p-regions. But the participation of heavy and light holes in the transport and a small energy separation between the levels of hole subbands complicate the phenomenon.

Results of numerical calculations of the D/μ ratio for electrons in n–i–p–i crystals based on GaAs are shown in Fig. 4. For $\sigma_c = 0$, the D/μ ratio would exhibit a saw-tooth-like dependence on ζ_e and n at low temperatures. Increasing the temperature



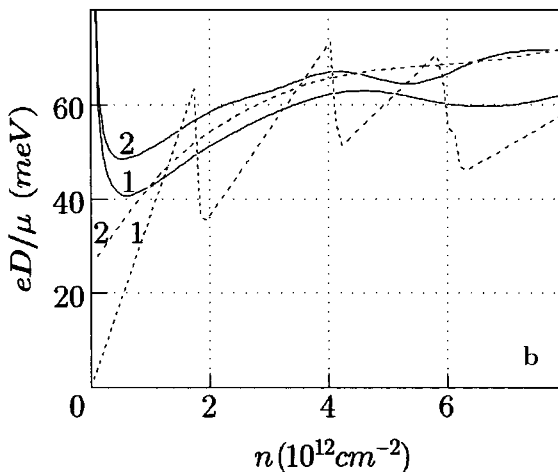


Fig. 4. The diffusivity–mobility ratio D/μ in the GaAs n–i–p–i crystal versus a) the chemical potential ζ_e and b) two-dimensional concentration n at the temperatures (1) $T = 4.2$ K and (2) 300 K. $N_a = 8 \times 10^{18}$ cm^{-3}, $N_d = 4 \times 10^{18}$ cm^{-3}, $d_n = d_p = 20$ nm, $d_i = 0$, $m_c = 0.067 m_e$, $\epsilon = 12.5$. The dashed curves correspond to the case of $\sigma_c = 0$. The solid ones represent effects of the density state tails

smoothes the dependencies and at room temperature quantization effects are not developed. But in the real case, where fluctuations of dopant concentrations are significant, the effect of reducing the density of state tails plays a major role. An anomalous behaviour of the D/μ ratio is to be observed in the electric quantum limit and at room temperature as well. The filling of high-lying subbands accompanied by the further reduction of the density of state tails results in an additional anomalous change of the value D/μ. The described anomalous changes of the D/μ ratio are larger in the n–i–p–i crystals than in bulk GaAs crystals [4] or ordinary quantum-well systems [10]. In any case the D/μ value exceeds the classical ratio kT/e.

At low pump intensities and for compensated n–i–p–i crystals the quasi-Fermi levels can drop deeply in the tail states and the spatial distribution of the current carriers becomes essentialy non-uniform. Therewith, the quantities D and μ are determined by the character of transport proceeses, but the relation between D and μ does not depend on the concrete scattering mechanisms [4, 12].

It is not astonishing that the diffusivity–mobility ratio belongs to one of the most important thermodynamical parameters of semiconductors and contributes to various characteristics and phenomena [13]. Doping superlattices represent a special member in the class of materials with anomalous features of the D/μ ratio. These features have to be taken into account in the analysis of performance of optoelectronic devices based on n–i–p–i crystals. Besides, the measuring of the D/μ ratio gives additional possibilities to examine design parameters of n–i–p–i crystals and the energy spectrum of confined carriers and to understand the role of the fluctuating impurity potential.

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