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Bipolar diffusion in two-dimensional structures

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Abstract

Spatial distribution of non-equilibrium carriers created by a partial interband illumination of two-dimensional structures was analyzed theoretically. Due to a weak electron screening in low-dimensional systems, the carrier distribution essentially differs from that in bulk semiconductors. Instead of exponential decay of quasi-neutral electron and hole concentration, the majority carrier distribution has a long-range hyperbolic tail, which can be either positive or negative, depending on the mobility ratio of majority and minority carriers.

Preface

The idea of this work came into being more than 10 years ago in our discussions with I.D. Vagner. We formulated the problem, the basic system of equations, and plans of further activity, which remained unimplemented for a long time being ousted by our independent activity in other fields. We returned to this problem only in 2006 but were stopped by the death of my friend and co-author. When the editors of the "Journal of Science and Engineering" approached me to make a contribution to this memorial issue, I decided to complete this work and present it as a memory of my old friend, world-class physicist, all-round gifted, nice, and kind personality – Israel Vagner.

A.Shik, Toronto, August 2007

1 Formulation of the problem

The problem of spatial distribution of non-equilibrium carriers in partially illuminated structures plays a central role in the theory of photoelectric phenomena. For interband optical excitation, the theoretical description of the effect is usually based on the quasi-neutrality concept, so that the distributions of electrons and holes assumed to coincide and are found from the diffusion equation with the effective ambipolar diffusion length L_a (see, e.g., [1]). Though this equation does not explicitly contain electrostatic forces, actually they play a key role since the concept of quasi-neutrality assumes that even small disbalance between the electron and hole concentrations creates strong electric field restoring quasi-neutrality. To be more exact, the profiles of non-equilibrium electrons and holes do not coincide absolutely but are shifted by the screening length r_s which in bulk samples is essentially less than L_a. This strong inequality justifies the assumption of quasi-neutrality.

The above-mentioned arguments are applicable to bulk semiconductor samples with all dimensions essentially exceeding r_s. In two-dimensional (2D) layers with the thickness $d \ll r_s$, the screening effects are much weaker (see, e.g., [2, 3]) and the deviations from local neutrality can be much more noticeable than in bulk samples. This may noticeably change all electronic properties caused by the sample illumination. Theoretical analysis of the diffusion of non-equilibrium carriers in 2D semiconductor structures is the main goal of the present work.

From the formal point of view, the basic difference between bulk and low-dimensional semiconductors consists in principally different approach used for the theoretical description of screening phenomena. In bulk semiconductors, all points of the sample where electric field has a non-zero value, contain free carriers moving in this field and providing effective screening. The resulting distribution of carrier density and electrical potential are found from the corresponding Poisson's equation. On the contrary, in 2D structures, electric field also exists in the whole surrounding space while free carriers are restricted in their motion to a single plane, which suppresses dramatically their screening ability. To find the potential distribution in this case, one should solve not the Poisson's but the Laplace equation in the whole space, where charges created by re-distribution of non-equilibrium carriers are taken into account in the boundary conditions to this equation, which will be performed below.

The results of this work have recently been developed and generalized to the case of monopolar photoconductivity, as well as to one-dimensional structures (semiconductor nanowires) [4].

1.1 General expressions

The central goal of the theory of non-equilibrium photoelectric phenomena consists in calculation of spatial distribution of the electrical potential φ and the concentrations of non-equilibrium electrons Δn and holes Δp. They should be found from the continuity equations:

$$\frac{\partial(\Delta n)}{\partial t} - \nabla \mathbf{j}_n/e = G - R_n; \tag{1}$$

$$\frac{\partial(\Delta p)}{\partial t} + \nabla \mathbf{j}_p/e = G - R_p; \tag{2}$$

$$\mathbf{j}_n = -\sigma_n \nabla\varphi(z=0) + eD_n\nabla(\Delta n); \tag{3}$$

$$\mathbf{j}_p = -\sigma_p \nabla\varphi(z=0) - eD_p\nabla(\Delta p). \tag{4}$$

Here G and $R_{n,p}$ are the generation and recombination rates, $\sigma_{n,p}$ and $D_{n,p}$ are the electron and hole conductivities and diffusion coefficients. We note that the system contains some amount of equilibrium carriers, which also contribute to recombination, so that, contrary to the generation rate, the electron and hole recombination rates in Eqs.(1),(2) can be different. We assumed that 2D electron gas occupies the plane $z = 0$. In this case $\Delta n, \Delta p$, as well as the current densities $\mathbf{j}_n, \mathbf{j}_p$, are functions of x and y, and all vectors, including the gradient ∇, have only x and y components. As to the potential φ, it depends on all three coordinates but for our purposes only its values at $z = 0$ are relevant. Eqs.(1)–(4) show no visual distinctions from similar expressions in a bulk sample, but have in fact different dimensionality. In 2D case Δn and Δp are the surface, rather than volume, densities, $\mathbf{j}_n$ and $\mathbf{j}_p$ are the linear current densities (measured, e.g., in the SI unit system in A/m), and $\sigma_{n,p}$ are the 2D conductivities.

What is principally different from the bulk case, is the connection between the potential and the local charge density, assigned to replace the Poisson's equation. As it was mentioned in Sec.1, it is the Laplace equation $\Delta\varphi = 0$, which in our case should be solved in the semi-space $z > 0$ with the boundary condition

$$\frac{\partial\varphi}{\partial z}(z=0) = \frac{2\pi e}{\varepsilon}[\Delta n - \Delta p]. \tag{5}$$

In Eq.(5) we have assumed that our 2D system is embedded into a medium with one single dielectric constant ε, which is typically a good approximation for heterostructures. If the dielectric constants at $z > 0$ and $z < 0$ differ, say, in the case of a thin film on a dielectric substrate, ε must be replaced

by $(\varepsilon_+ + \varepsilon_-)/2$ [2]. Eq.(5) can be also generalized to the case of MOS and heterostructures with a metal gate by adding the term describing image forces.

Note that for our theory to be valid, it is not required that both types of carriers are truly 2D with strongly quantized energy spectra in z-direction. The only necessary condition is that all characteristic lengths in the xy-plane to be obtained from the solution of our equations, exceed considerably the electron and hole confinement lengths in z-direction. If, besides, electron and holes are separated by the built-in contact electric field at some distance in z-direction, this distance must be also much less than the above-mentioned characteristic diffusion lengths.

For further analysis we assume, as it is usually done for interband photoexcitation [5], the linear character of recombination: $R_n = \Delta n/\tau$, $R_p = \Delta p/\tau$. In this case, the system Eqs.(1)-(4) in the stationary case can be reduced to the system

$$\frac{1}{e}(\sigma_n + \sigma_p)\nabla^2\varphi(z=0) - D_n\nabla^2(\Delta n) + D_p\nabla^2(\Delta p) = \frac{1}{\tau}(\Delta p - \Delta n); \quad (6)$$

$$\sigma_p D_n\nabla^2(\Delta n) + \sigma_n D_p\nabla^2(\Delta p) = \frac{1}{\tau}(\sigma_p\Delta n + \sigma_n\Delta p) - G(\sigma_n + \sigma_p). \quad (7)$$

We have linearized the equations neglecting the dependences of $\sigma_{n,p}$ on Δn and Δp.

2 Stationary distribution of electrons and holes

The problem can be solved relatively simple for a strongly extrinsic systems with electron and hole conductivities differing drastically, for example, at $\sigma_n \gg \sigma_p$. In this case Eq.(7) gives

$$D_p\nabla^2(\Delta p) = \frac{\Delta p}{\tau} - G \quad (8)$$

which means that the minority carrier motion is not influenced by Coulomb forces and comprises a pure diffusion with the coefficient D_p. In the case of semi-illuminated sample: $G = G_0$ at $x < 0$; $G = 0$ at $x > 0$,

$$\Delta p(x) = G_0\tau\left[1 - \frac{1}{2}\exp(x/L_p)\right],\ x < 0;$$
$$\Delta p(x) = \frac{G_0\tau}{2}\exp(-x/L_p),\ x > 0 \quad (9)$$

where $L_p = \sqrt{D_p \tau}$.

Then the distributions of a surface charge $q = e(\Delta p - \Delta n)$ and of an electrostatic potential $\varphi(z = 0)$ can be found. If we take into account that $\varphi(z = 0)$ is connected with q by the expression similar to Eq.(**??**), than for a planar hole distribution depending on one coordinate x (given, e.g., by Eq.(9)), Eq.(6) gives:

$$D_n q''(x) - \frac{q(x)}{\tau} - \frac{4\sigma_n}{\varepsilon} \int_0^\infty \lambda \sin(\lambda x) \int_0^\infty q(t) \sin(\lambda t)\, dt d\lambda = e(D_n - D_p)(\Delta p(x))'' \tag{10}$$

where $\Delta p(x)$ is given by Eq.(9). Since the right side of Eq.(10) is odd in x, then $q(x)$ also should be odd. Multiplying Eq.(10) by $\sin(\mu x)$ and integrating over x, we obtain the equation for $\widetilde{q}(\kappa) = \int_0^\infty q(x) \sin\left(\frac{\kappa x}{L_n}\right) \frac{dx}{L_n}$:

$$\widetilde{q}(\kappa)\left(\kappa^2 + 2A\kappa + 1\right) = -\frac{eG_0\tau\,(1-b)\,\kappa}{2(1+b\kappa^2)} \tag{11}$$

which after the inverse Fourier transform gives

$$q(x) = -\frac{eG_0\tau(1-b)}{\pi} \int_0^\infty \frac{\kappa \sin(\kappa x/L_n)\, d\kappa}{(\kappa^2 + 2A\kappa + 1)(b\kappa^2 + 1)}. \tag{12}$$

Here $A = \pi\sigma_n\tau/(\varepsilon L_n)$, $L_n = \sqrt{D_n\tau}$, $b = D_p/D_n$.

The spatial distribution of non-equilibrium charge density $q(x)$ depends on the parameters b and A. The first of them characterizes asymmetry of the electron-hole system, which causes the emerging of all electrostatic phenomena discussed in this paper. At $b = 1$ both electrons and holes are distributed in accordance with Eq.(9), local neutrality is maintained and no difference with bulk samples occurs. At $b < 1$ electrons are more mobile than holes, so that $q(x)$ is negative in the non-illuminated region $x > 0$ and positive at $x < 0$. At $b > 1$ the picture is opposite.

The exact shape of distribution is determined by A, which characterizes the relative intensity of drift and diffusion transport. At $A \ll 1$ carrier drift is of a minor importance, so that $q(x)$ at $x > 0$ is a superposition of the hole density given by Eq.(9) and the similar expression for the electron density:

$$q(x) = \frac{eG_0\tau}{2} \left[\exp(-x/L_p) - \exp(-x/L_n)\right]. \tag{13}$$

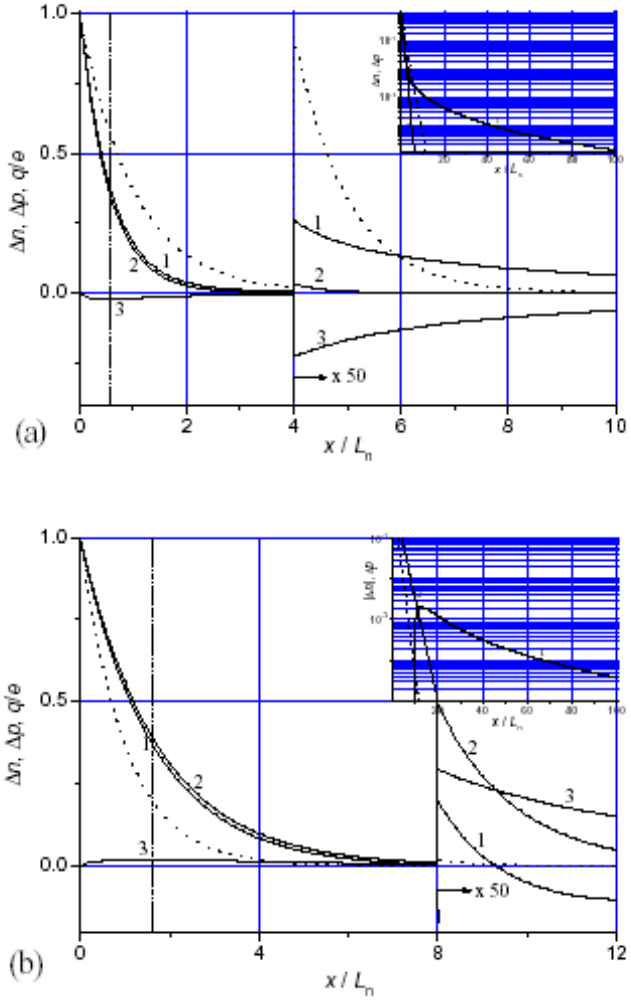

Figure 1: Spatial distribution of the electron concentration Δn (1), the hole concentration Δp (2), and the surface charge $q = e(\Delta p - \Delta n)$ (3) created by the bipolar injection from illuminated region at $A = 10$ for $b = 0.3$ (a) and $b = 3$ (b) in 2D systems. The dotted line shows the dependence $\Delta n \sim \exp(-x/L_n)$. At $x > 4L_n$ (a) or $x > 8L_n$ (b) the vertical scale is increased. $\Delta n, \Delta p$, and q/e are measured in the units $eG_0\tau$. Vertical dash-and-dot lines show the value of L_p. The inserts show the same concentration profiles in the semi-logarithmic scale. Since in the case (b) Δn at large x is positive, the curve 1 at the corresponding insert shows $|\Delta n|$.

At $A \gg 1$ the decay of $\Delta n(x)$ and $q(x)$ is strongly modified by Coulomb effects, which is illustrated by Fig.1. At relatively small x, the spatial distribution of electrons for any b almost coincides with that of holes, similarly to the bulk samples. However, the tail of electron and charge distribution is essentially different from the three-dimensional case and depends on the value of b.

For $b < 1$ (majority carriers are more mobile) the concentration of non-equilibrium electrons at large x decays much slower than the exponential function $\exp(-x/L_n)$. Such a tail, which is seen especially clear at the insert in Fig.3a, reminds hyperbolic charge tails occurring in other 2D electrostatic problems [2, 3, 6] and has the same physical origin. For $b > 1$ (minority carriers are more mobile) the long-range tail has a positive, rather than negative, charge and is caused by removal of some amount of equilibrium electrons.

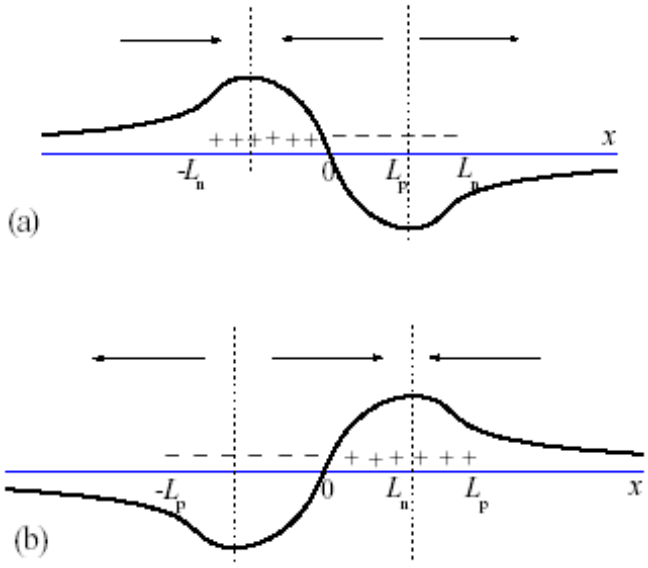

Figure 2: Schematic distribution of the electrical potential in a 2D layer with bipolar injection for $b < 1$ (a) and $b > 1$ (b). Pluses and minuses near the axis show the surface charge sign in the given region. Arrows show the direction of electron drift.

The mentioned features differing from the characteristics of bipolar diffusion in bulk materials are related to the specific properties of electric potential created by a planar charge distribution. Simple calculations show that two neighboring coplanar stripes of positive and negative surface charges create, contrary to the bulk double charged layer, a non-monotonic potential distribution shown schematically in Fig.2. While the spatial distribution of minority carriers (holes) is fixed and given by Eq.(9), the distribution of non-equilibrium electrons is determined by the joint influence of diffusion and drift in the above-mentioned potential. The direction of this drift is shown by arrows in Fig.2 and explains the observed deviations of $\Delta n(x)$ from the exponential distribution $\exp(-x/L_n)$ shown for comparison by dotted lines in Fig.1. These deviations include the the conforming of $\Delta n(x)$ with $\Delta p(x)$ at small x and long tails at large x caused by accumulation (at $b < 1$) or extraction (at $b > 1$) of electrons by the self-consistent electric field.

3 Kinetics of carrier distribution

Let us consider the relaxation of the described bipolar carrier distribution after turning off the light excitation. Similarly to the stationary case considered above, the equation for minority carriers splits off and gives

$$\frac{\partial(\Delta p)}{\partial t} = D_p \nabla^2(\Delta p) - \frac{\Delta p}{\tau}. \tag{14}$$

Its solution for the initial condition Eq.(9) is

$$\Delta p(x,t) = \frac{G_0\tau}{2}\left[\exp\left(-\frac{t}{\tau}\right) - \frac{2}{\pi}\int_0^\infty \sin\left(\frac{\lambda x}{L_p}\right)\exp\left(-\frac{(1+\lambda^2)t}{\tau}\right)\frac{d\lambda}{\lambda(1+\lambda^2)}\right]. \tag{15}$$

Similarly, the non-stationary analog of Eq.(10) has the form

$$D_n\frac{\partial^2 q(x,t)}{\partial x^2} - \frac{\partial q(x,t)}{\partial t} - \frac{q(x,t)}{\tau} - \frac{4\sigma_n}{\varepsilon}\int_0^\infty \lambda\sin(\lambda x)\int_0^\infty q(\xi,t)\sin(\lambda\xi)\,d\xi d\lambda$$
$$= e(D_n - D_p)\frac{\partial^2[\Delta p(x,t)]}{\partial x^2}. \tag{16}$$

Substituting Eq.(15) into the right side of Eq.(16), we obtain the equation for $\widetilde{q}(\kappa,t) = \int_0^\infty q(x,t)\sin\left(\frac{\kappa x}{L_n}\right)\frac{dx}{L_n}$:

$$\widetilde{q}(\kappa,t)\left(\kappa^2+2A\kappa+1\right)=-\tau\frac{\partial\widetilde{q}(\kappa,t)}{\partial t}-\frac{eG_0\tau(1-b)\kappa}{2(1+b\kappa^2)}\exp\left[-\frac{(1+b\kappa^2)t}{\tau}\right] \tag{17}$$

generalizing Eq.(11) to the non-stationary case. Eq.(17) can be easily solved using $\widetilde{q}(\kappa)$ determined by Eq.(11) as the initial condition $\widetilde{q}(\kappa,0)$. The inverse Fourier transform gives the final expression for kinetics of the charge distribution:

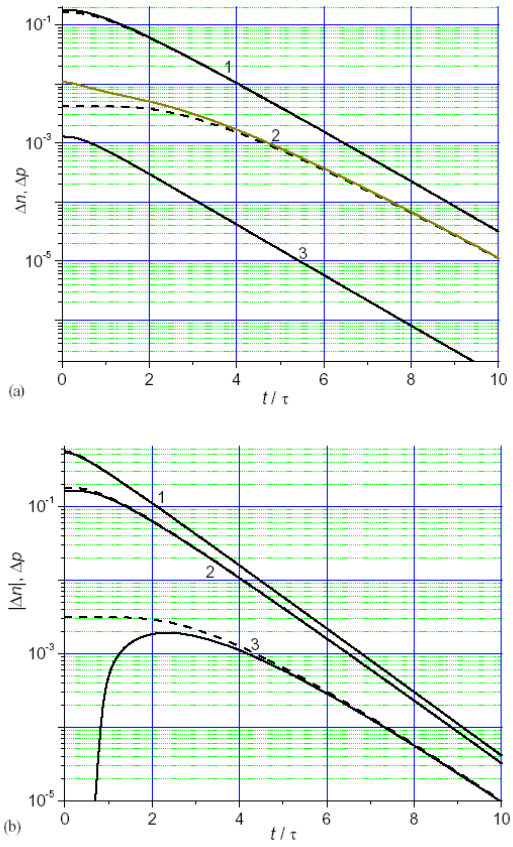

Figure 3: Relaxation kinetics of electrons (solid lines) and holes (dashed lines) at $A = 10$ for $b = 0.3$ (a) and $b = 3$ (b) in 2D systems at: 1 – $x = L_n$; 2 – $x = 3L_n$; 3 – $x = 10L_n$. For $b < 1$ the value of Δp at $x = 10L_n$ is too small and the corresponding curve lies beyond the graph.

$$q(x,t) = -\frac{eG_0\tau(1-b)}{\pi}\left\{\int_0^\infty \frac{\sin(\kappa x/L_n)\exp\left[-\frac{(1+b\kappa^2)t}{\tau}\right]d\kappa}{[(1-b)\kappa+2A](b\kappa^2+1)}\right. \quad (18)$$
$$\left. -\int_0^\infty \frac{\sin(\kappa x/L_n)\exp\left[-\frac{(\kappa^2+2A\kappa+1)t}{\tau}\right]d\kappa}{[(1-b)\kappa+2A](\kappa^2+2A\kappa+1)}\right\}.$$

Fig.3a shows the relaxation kinetics of Δp (given by Eq.(15)) and Δn (obtained from Eqs.(15) and (18)) in three different points of a sample for the case $b < 1$ (majority carriers have higher mobility). At small x (curves 1) where quasi-neutrality is maintained, electrons and holes relax synchronously. At intermediate x (curves 2), Δp remains almost constant during the initial decay of Δn until these concentrations match, after which their relaxation continues synchronously. Finally, at large x belonging to a long tail of Δn, the concentration of holes is negligibly small, so that we can speak of individual relaxation of Δn. For this reason, Fig.3a has no dashed curve 3 at all since the corresponding dimensionless Δp at $x = 10L_n$ even at the initial moment has the order of 10^{-8}. In the case $b > 1$ (Fig.3b) the most remarkable feature of the long tail is the change of sign of Δn in the course of relaxation.

4 Conclusion

It was shown that in low-dimensional structures suppression of the screening effect due to the confinement of electron motion essentially changes diffusion processes in a system of optically induced carriers. In bipolar diffusion, due to a non-monotonic potential distribution in low-dimensional systems (Fig.2), drift effects in some cases do not restore but rather destroy quasi-neutrality. The best demonstration of this phenomenon is the occurrence of a long tail in the distribution of non-equilibrium majority carriers shown in the inserts in Fig.1.

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