Interface recombination feature in metal–semiconductor junction at high photo-excitation

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Abstract

A theory of the photo-induced electromotive force in a p-type semiconductor accounting for the energy band bending and interface recombination dependence on excitation level is developed. It is shown that at high photo-excitation the effective interface recombination velocity in the metal-semiconductor junction is negligible compared with the volume one, when the surface potential is less than its critical value. The photo-induced electromotive force value is maximal at this condition.

Keywords: continuity equations, Poisson equation, diffusion length, interface recombination, photo-induced electromotive force

1. Introduction

The recombination of the nonequilibrium (NE) carriers in the bulk and in the surfaces/interfaces of the semiconductor structure plays an important role in transport phenomena. There are many effects, the values of which depend considerably on the interface recombination: photoconductivity [1], photo-induced electromotive force (EMF), magnetococoncentration effect [2] and so on. Typically used expression of the surface recombination velocity (the Stevenson–Keyes theory) is obtained in quasi-neutrality approximation and assumption of small carrier concentrations’ deviation from those of the equilibrium. According to this theory the surface recombination velocity significantly depends on the band bending [1, 3]. Though measurements of the interface recombination velocity [5–7] are based on the quasineutrality model [3], the criterion of low excitation as a rule is not fulfilled. As it is shown in [4] the expression of the surface recombination velocity of the Stevenson–Keyes theory is invalid at high excitation levels. In general, the surface recombination rate has the form [4] 

\[ R_s = S_n \delta n_s + S_p \delta p_s \]

where \( S_n, S_p \) are the interface recombination parameters and \( \delta n_s, \delta p_s \) is the NE electron (hole) concentration in the interface. This expression of the surface recombination rate allows us to eliminate contradiction of the classical Hall electric field generation model related to the NE surface charge layer, which does not depend on the interface recombination value [4]. The expressions of the interface recombination parameters \( S_n \) and \( S_p \) at any NE carrier value are derived in [4], and use the Shockley–Read model for the interface recombination. The experimental data corroborates the interface recombination theory [4]. The interface recombination rate is equal to \( R_s = S_p \delta p_s \) [8, 9] in the metal–semiconductor junction (MSJ), because there are no NE electrons in the MSJ (\( \delta n_s = 0 \) owing to the constancy of metal chemical potential and continuity of electrical potential). As follows from the results of [4], the interface recombination parameter \( S_p \) decreases, thus increasing the excitation level. This effect is strongly expressed in the junction of a metal and p-type semiconductor at high photo-excitation. In this case the interface recombination can become less than the bulk recombination in a certain region of the surface potential (SP) [3] value. The influence of the interface recombination on the photo-induced EMF can be negligible in this SP region.
This paper is aimed at the study of the surface potential influence on the interface recombination in the MSJ at high photo-excitation levels.

2. Theory

In order to study the interface recombination feature let us consider the photo-induced EMF generation. Let us consider a p-type non-degenerate semiconductor plate $0 \leq x \leq a$ with the surface at $x = 0$ illuminated by strongly absorbed light. The thickness of the sample $a$ essentially exceeds the diffusion length. A semitransparent thin metallic film is placed on the surface $x = a$. Interface recombination is extremely large on the surface $x = a$.

The NE densities of electrons $\delta n$ and holes $\delta p$, as well as the NE electric potential $\phi_m$, are obtained from solution of the continuity equations [10, 11] and the Poisson equation

$$\frac{1}{e} \frac{dj_n}{dx} - \frac{\delta n}{\tau_n} - \frac{\delta p}{\tau_p} = 0,$$

$$\frac{1}{e} \frac{dj_p}{dx} + \frac{\delta n}{\tau_n} + \frac{\delta p}{\tau_p} = 0,$$

$$\frac{d^2 \delta p}{dx^2} = - \frac{\delta p}{\epsilon \varepsilon_0},$$

where $-e$ is the electron charge, $j_n$, $j_p$ are the electron and hole current densities, $\tau_n$ ($\tau_p$) is the parameter characterizing electron (hole) bulk recombination velocity, $\delta p$ is the NE charge density, $\varepsilon$ is the semiconductor electrical permittivity, and $\varepsilon_0$ is the vacuum permittivity.

The expressions for $x$-component of partial currents are [3]:

$$j_n = -e\mu_n \frac{dp}{dx} + \mu_n kT \frac{dn}{dx},$$

$$j_p = -e\mu_p \frac{dp}{dx} - \mu_p kT \frac{dp}{dx},$$

where $\mu$ ($\mu_e$) is the electron (hole) mobility, $n(x)$, $p(x)$ are the densities of electron and hole accordingly, $\phi$ is the electric potential, $k$ is the Boltzmann constant, and $T$ is the temperature of the semiconductor.

The boundary conditions in the MSJ are obtained in [8, 9]:

$$e^{-i \gamma} j_n(0) = S_p \delta p(0) - G,$$

$$\delta n(0) = 0,$$

$$\delta q_m = \delta \phi(0),$$

where $S_p$ is the interface recombination parameter, $\delta q_m$ is the NE electric potential of the metallic contact, and $G$ is the electron-hole pair (EHP) surface generation rate. It follows from equation (5) and the results of [4] that parameter $S_p$ is not the surface recombination velocity of the holes. The validity of boundary condition (6) is proved in [12], which studies the role of the NE charge in the thermopower generation.

In the most of semiconductors the diffusion length $\lambda$ significantly exceeds the Debye length $\lambda_D$ [8]. Under this condition the solution of equations (1)–(4) could be obtained in the following way. Let us consider the virtual surface $x = l$, where $l = (5 \div 8) r_p$. The Debye (D) mode is the solution of equations (1)–(4) in the region $0 \leq x \leq l$ and the recombination (R) mode is the solution of equations (1)–(4) in the quasi-neutrality region $l \leq x \leq a$. The R mode and the D mode are denoted by subscripts $r$ and $d$ accordingly. The NE carrier concentrations are continuous in the virtual surface. The NE electric potential is equal to the sum of the NE electric potentials of the D and the R modes. The photo-excitation is high, if the EHP concentration satisfies the condition $n_0 \ll \delta n_r, \ll p_0$.

The R mode satisfies the total current continuity equation $j_n + j_p = 0$ and the diffusion equations [2, 3]

$$\frac{d^2 \delta n_r}{dx^2} = - \frac{\delta n_r}{\epsilon \varepsilon_0},$$

where $\lambda = \sqrt{D_l \lambda_n}$ is the diffusion length of the EHP, $\tau_n$ is the lifetime of the EHP in the bulk of a p-type semiconductor sample [2, 11] and $D_l = kT \phi_m/e$ is the diffusion coefficient of the electrons. As follows from [2, 8] in a p-type semiconductor the diffusion coefficient of the EHP coincides with one of the electrons. The density of holes $\delta p$ satisfies equation (8) too since in the quasi-neutrality region the equality $\delta q_m = \delta \phi_r$ is valid. Note that the lifetime of the EHP in the bulk of the sample $\tau_n$ is constant at $\delta n_r \ll p_0$ [3, 11].

We obtain for the R mode:

$$\delta n_r = \delta n_r(l) \exp \left( - \frac{x}{\lambda} \right)$$

The D mode satisfies the equations [8]

$$\frac{dj_n}{dx} = 0, \quad \frac{dj_p}{dx} = 0$$

because we can neglect the bulk recombination in the region $0 \leq x \leq l$ accounting for the inequality $n_0 \ll \lambda$.

Solving equations (4), (10) we obtain the relations between the carrier densities and the electric potential of the D mode [12]:

$$\delta n_d = n_r \left[ 1 + \frac{\delta n_r(l)}{n_0} \exp \left( \frac{e \delta \phi_d}{kT} \right) - 1 \right],$$

$$\delta p_d = p_r \left[ 1 + \frac{\delta n_r(l)}{p_0} \exp \left( - \frac{e \delta \phi_d}{kT} \right) - 1 \right],$$

where $n_r$, $p_r$ are the equilibrium densities of electrons and holes in the region $0 \leq x \leq l$ and $n_0$, $p_0$ are the equilibrium densities of the ones in the bulk of the sample.
The expression of the interface recombination parameter $S_p$ has the form [4]
\[
S_p = \frac{\alpha_{ns}\alpha_{ps}n_{is}}{\alpha_{ns}(n_{es} + n_{ih}) + \alpha_{ps}(p_{es} + p_{1h} + \delta n_{i})}
\] (13)
where $\alpha_{ns}(\alpha_{ps})$ is the capture coefficient of electrons (holes), $N_{is}$ is the total density of interface impurity states, $\delta n_{i}$ is the NE hole concentration in the interface, the $n_{ih}(p_{1h})$ is the electron (hole) concentration in the surface when the Fermi level matches the activation energy of the interface trapping level [4], $n_{es} = n_0 \exp (-eq_{es}/kT)$ is the equilibrium concentration of electrons in the interface, $p_{es} = p_0 \exp (-eq_{es}/kT)$ is the equilibrium concentration of holes in the interface and $q_{es}$ is the equilibrium SP. Accounting for equations (6), (11) and (12) we can also rewrite BC (5)
\[
e^{-\frac{i}{j_p}}(0) = S_{ef} \delta n_{i}(l) - G
\] (14)
where $S_{ef} = S_{f}p_{es}/n_0$ is the effective interface recombination velocity (IRV).

We derive from equations (13) and (14):
\[
\delta n_{i}(l) = 0.5n_0A^{-1}\left(-B + \sqrt{B^2 + 4A\frac{G\lambda}{n_0D_{hi}}}\right)
\] (15)
where $S_0 = \alpha_{ns}N_{is}$ is the IRV at low photo-excitation ($\delta n_{i}(l) \ll n_0$) and flat energy band,
\[
A = \alpha_{ns}(n_{es} + n_{ih}) + \alpha_{ps}(p_{es} + p_{1h})
\]
\[
B = 1 + A\frac{\lambda}{D_{hi}}\left(S_0 \exp \left(\frac{eq_{es}}{kT}\right) - \frac{G}{\eta_0}\right).
\]

After some mathematical manipulations we obtain the general expression of the photo-induced EMF
\[
U_p = -\frac{kT}{e} \ln \left(1 + \frac{\delta n_{i}(l)}{n_0}\right).
\] (16)

The developed model is valid under condition $\alpha \gg \lambda^{-1}$ and $\lambda \gg \eta_0$, where $\alpha$ is the light absorption coefficient.

3. Discussion of results

It follows from equations (14) and (15) that at high photo-excitation level the effective IRV is negligible compared with the volume one if the SP is less than the critical value $q_{es}^{cr} = (kT/e) \ln \left(G/10n_0S_0\right)$. The photo-induced EMF modulus is maximal in this SP region
\[
\left|U_p\right|_{\text{max}} = \frac{kT}{e} \ln \left(1 + \frac{G\lambda}{n_0D_{hi}}\right).
\]

This effect is caused by strong growth of the NE holes’ concentration in the interface, which significantly diminishes the effective IRV value at $q_{es} \lesssim q_{es}^{cr}$.

The effective IRV dependence on the equilibrium SP in $p$-Si ($T = 293 K$, $p_0 = 4 \times 10^{19} \text{cm}^{-3}$, $A = 0.06 \text{cm}^2$ [13, 14], $p_{0i} = 1450 \text{cm}^2 \text{V}^{-1} \text{s}^{-1}$, $G = 10^{10} \text{cm}^{-2} \text{s}^{-1}$) for some $S_0$ values is shown in figure 1. We suppose that in Si the trapping level is near the middle of the band gap [1] owing to the wide one ($E_g = 1.12 \text{eV}$). In Si the condition $\alpha \gg \lambda^{-1}$ satisfies with a great accuracy at the light wavelength less than 900 nm [15]. The IRV smallness condition $S_{ef} << D_{hi}/\lambda = 609 \text{cm}^{-1}$ holds at $q_{es} \lesssim q_{es}^{cr} = 0.37 \text{eV}$. Note that according to the Stevenson–Keyes theory, the maximum of the interface recombination velocity occurs at $q_{es} = 0.3 \pm 0.32 \text{eV}$ and it is $5 \times 10^4$ times higher than the $S_0$ value. The photo-induced EMF dependence on the equilibrium SP is shown in figure 2. It is seen that $U_p = -0.47 \text{V}$ at $q_{es} \lesssim 0.37 \text{V}$ in a wide region of the $S_0$ value ($S_0 \lesssim 5 \times 10^3 \text{cm} \cdot \text{s}^{-1}$). Considering the semiconductor this effect is expected at $G = (10^{13} \div 10^{16}) \text{cm}^{-2} \text{s}^{-1}$ and $q_{es} \lesssim 0.31 \text{V}$.

Thin aluminum film can be used as the conductive and semitransparent to the light contact placed on the illuminated
semiconductor surface. The equilibrium SP exceeds 0.45 V in the typically used Al/p-Si junction. However it is known [1] that the SP of the semiconductor very largely depends on the surface level density. If we create the sufficient density of the acceptor-type surface levels, we can make the SP value less than 0.37 V.

4. Conclusions

The effective IRV dependence on the surface potential in the contact of a metal and p-type semiconductor at high photo-excitation level is studied. It is shown that the effective IRV in the MSJ is negligible compared with the volume one in a certain band bending region. The photo-induced EMF is maximal in the same SP region. The experimental verification of the theory is discussed.

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