Modelling of asymmetric n-p junction enriched with charge carriers in equilibrium state

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Abstract. Modelling n-p-junction is an urgent task, because theoretical models do not describe all the properties of semiconductor structures with different content of impurities. The influence of impurities on the properties of asymmetric n-p-junction was analyzed in the paper. The Poisson equation in the space charge region (SCR) of the equilibrium n-p-junction was solved numerically. The charge density in the SCR was also calculated. It has been shown that the structure of SCR of strongly asymmetric n-p-junction substantially differs from the model of depleted charge carriers, and includes four parts: 1 – highly doped region, wherein the main charge carriers partially compensate the charge of the ionized impurities; 2 – low-doped region containing ionized impurities of the opposite sign with respect to the first, enriched with charge carriers, increasing the charge of ionized impurities; 3 – lowly doped region, wherein the concentrations of electrons and holes much less than the concentration of ionized impurities; 4 – lowly doped region, wherein the main charge carriers partially compensate the charge of the ionized impurities.

1. Introduction

A correct description of an n-p junction is necessary for solving applied problems and determining the parameters of semiconductor devices [1, 2]. The asymmetry of the potential barrier of a front close-lying n-p junction makes it difficult to determine the parameters of the space-charge region of real semiconductor structures. Experimental data [3] indicate the influence of the surface charge on the potential barrier value and space charge region (SCR) parameters of the structures with a front close-lying asymmetric diffusion n-p junction.

The theory of semiconductor devices with an n-p junction, formulated by Shockley [4], is continuously being improved. Popularity was obtained by models describing two limiting cases [5, 6]: an abrupt n-p-junction, a graded n-p-junction with a linear distribution of impurities. Numerical models have been developed for n-p-junctions with a real impurity profile.

The key point of the theory of n-p junction is the existence of a region depleted of charge carriers, in which the concentration of electrons and holes is much less than the concentration of dopant impurities [4]. Accounting for the concentration of charge carriers made it possible to more accurately calculate the size of the space charge region (SCR) [5, 6]. The numerical models are used in the case of a strongly asymmetric n-p junction, as well as a front close-lying one [7-9].

The relevance of modelling the n-p junction has not lost its significance at the present time [10, 11]. It was shown in [12] that the distribution of electron and hole concentrations in an equilibrium abrupt n-p junction corresponds to the model of the SCR depleted of charge carriers, widely used to
analyze semiconductor devices [13, 14]. However, the distribution of charge carrier concentration in a strongly asymmetric diffusion n-p junction is not described by this model [9].

The aim of the work is to prove that in the SCR of a strongly asymmetric diffusion n-p junction there is a region enriched with charge carriers.

2. Modelling of charge carrier distribution in diffusion n-p junction

The model is based on the system of equations formulated by Shockley [4] for semiconductors with homojunctions. In the stationary one-dimensional case, this system of equations is of the following form:

\[
\begin{align*}
\frac{d}{dx} j_n &= \mu_n n \frac{d}{dx} \varphi - D_n \frac{d}{dx} n \\
\frac{d}{dx} j_p &= -\mu_p p \frac{d}{dx} \varphi - D_p \frac{d}{dx} p \\
\frac{d}{dx} j_n &= G - R \\
\frac{d}{dx} j_p &= G - R \\
\frac{d^2}{dx^2} \varphi &= -\frac{q}{\varepsilon \varepsilon_0} (p - n + N)
\end{align*}
\]

(1)

where \( j_n, j_p \) are the flux densities, \( \mu_n, \mu_p \) are the mobilities, \( n, p \) are the concentrations, \( D_n, D_p \) are the diffusion constants for electrons and holes, respectively, \( \varphi \) is the electrical potential, \( G, R \) are the rates of bulk generation and bulk recombination of electron-hole pairs, \( q \) is the elementary electric charge, \( \varepsilon \) is the permittivity, \( \varepsilon_0 \) is the dielectric constant, \( N \) is the function of the distribution ionized impurities concentrations.

The distribution of ionized impurities creating a front close-lying asymmetric diffusion n-p junction is described by the following formula

\[
N(x) = N_{D0} \text{erfc}(x / x_1) - N_A,
\]

(2)

where \( N_{D0} \) is the concentration of ionized donors on the front surface, \( x_1 \) parameter defines the depth of the n-p junction \( w_a \).

Numerical solution of the system of equations (1) with boundary conditions on the front and back surfaces for the front diffusion n-p junction in silicon under solar illumination is shown in the figure 1.

The calculated distribution of the electron and hole concentrations at different values of the contact voltage \( U \) shows that the metallurgical boundary located at \( x = 0.2 \mu \text{m} \) is surrounded by a region enriched with electrons. There are 3 regions in the illuminated front close-lying asymmetric diffusion n-p junction:

- the 1st one is the emitter containing a positive charge density lower than the concentration of ionized donors, so that \( n \approx N \);
- the 2nd one is the region enriched with electrons, in which the electron concentration exceeds the concentration of ionized impurities, \( n > |N| \);
- and the 3rd region is the region depleted of electrons and holes containing the negative charge density created by ionized acceptors. The size of the region enriched with electrons increases with increasing \( U \) voltage. The hole distribution at \( U = 0 \) has a local maximum near the front surface due to the influence of surface recombination.
Figure 1. Concentrations of ionized impurities $N$, electrons $n$ and holes $p$ in the diffusion $n$-$p$ junction at different $U$ voltage values. 1: $|N(x)|$; 2: $n(x)$ at $U = 0$; 3: $n(x)$ at $U = 0.5$ V; 4: $p(x)$ at $U = 0$; 5: $p(x)$ at $U = 0.5$ V.

For the final conclusion on the presence of a region enriched with charge carriers, in the SCR of the $n$-$p$ junction we exclude the possible influence of the shape of the diffusion distribution of impurities and illumination. To do this, we numerically calculate the distribution of electrons and holes in the abrupt $n$-$p$ junction in an equilibrium state.

3. Numerical solution of the Poisson equation for an abrupt equilibrium $n$-$p$ junction

Let’s consider an abrupt $n$-$p$ junction. The SCR is located at $-d_n \leq x \leq d_p$. The concentrations of ionized donors $N_D(x)$ and acceptors $N_A(x)$ are given in the form of step functions:

$$N_D(x) = \begin{cases} 0, & -w_s \leq x < 0 \\ N_d, & 0 \leq x \leq w_p \\ N_D, & -w_s \leq x \leq 0 \\ 0, & 0 < x \leq w_p \end{cases}$$

$$N_A(x) = \begin{cases} 0, & -w_s \leq x < 0 \\ N_A, & 0 \leq x \leq w_p \\ N_A, & -w_s \leq x \leq 0 \\ 0, & 0 < x \leq w_p \end{cases}$$

(3)

The concentrations of equilibrium electrons $n(x)$, holes $p(x)$ are defined by the formulas [5, 6]:

$$n(x) = N_c e^{\frac{F - F_E + \phi(x)}{kT}},$$

$$p(x) = N_c e^{\frac{F - E_g + \phi(x)}{kT}},$$

(4)

where $N_c$ is the effective density of electronic states in the vicinity of the bottom of the conduction band, $F$ is the electrochemical potential (Fermi level) counted from the top of the valence band at the point $x = w_p$, $q$ is the elementary electric charge, $\phi(x)$ is the potential of the internal electric field, $k$ is the Boltzmann's constant, $T$ is the absolute temperature, $N_c$ is the effective density of electronic states in the vicinity of the top of the valence band, $E_g$ is the energy bandgap.

The potential of the internal electric field is a solution of the Poisson equation [5, 6]:

$$\frac{d^2 \phi}{dx^2} = -\frac{N_D - N_A}{\varepsilon}$$

where $\varepsilon$ is the permittivity of the semiconductor.
\[
\frac{d^2 \phi(x)}{dx^2} = -\frac{q}{\varepsilon \varepsilon_0} \left(p(x) - n(x) + N_D(x) - N_A(x)\right).
\]  
(5)

An additional condition for the equation (5) is the condition of total electroneutrality [5, 6]:

\[
\int_{-w_n}^{w_p} (p(x) - n(x) + N_D(x) - N_A(x)) dx = 0,
\]  
(6)

In general, the charge is distributed over the entire length of the semiconductor at \(-w_n < x < w_p\), so that the parameters \(d_n, d_p\) do not enter into the equations explicitly. In the structure under consideration, the charge density on the external surfaces is absent, therefore

\[
p(-w_n) - n(-w_n) + N_D = 0, \quad p(w_p) - n(w_p) - N_A = 0.
\]  
(7)

For an ideal plane-parallel structure, it follows from (6, 7) that

\[
\frac{d}{dx} \phi(x) \bigg|_{x=-w_n} = \frac{d}{dx} \phi(x) \bigg|_{x=w_p} = 0.
\]  
(8)

The discontinuity of the distributions \(N_D(x)\) and \(N_A(x)\) (3) at \(x = 0\) causes a discontinuity of the second derivative \(\phi(x)\). Equation (5) was solved in the regions \(-w_n \leq x < 0\) and \(0 \leq x \leq w_p\), the solutions were stitched at \(x = 0:\)

\[
\phi(x) \bigg|_{x=0} = \phi(x) \bigg|_{x=0}, \quad \frac{d}{dx} \phi(x) \bigg|_{x=0} = \frac{d}{dx} \phi(x) \bigg|_{x=0}.
\]  
(9)

For given \(N_c, N_v, E_g, q, k, T, \varepsilon, \varepsilon_0, N_D, N_A, w_n, w_p\), we find the potential of the internal electric field \(\phi(x)\) at \(-w_n \leq x \leq w_p\) as a numerical solution of the equation (5) with the boundary condition \(\phi(-w_n)\) and \(\phi(w_p) = 0\), where \(\phi(-w_n)\) and \(F\) are the roots of equations (7).

The calculated dependence of \(\phi(x)\) and the formulas (3, 4) were used to determine the charge density

\[
\rho(x) = p(x) - n(x) + N_D(x) - N_A(x).
\]  
(10)

As a result, the charge density in a silicon \(n-p\) junction at \(T = 300\) K is calculated. The parameters \(N_c, N_v, E_g, \varepsilon\) are given in [5, 6]. The distribution of charge density in an abrupt, symmetric \(n-p\) junction is shown in the figure 2, while in an abrupt, asymmetric \(n-p\) junction it is shown in the figure 3. The charge density \(\rho(x)\) is normalized to the value of \(N_D\) in the \(n\)-region and to the value of \(-N_A\) in the \(p\)-region to represent it on a single scale.

In the region depleted of charge carriers, \(n, p \ll N_D, n, p \ll N_A\), therefore

\[
\frac{\rho(x)}{N_D} \approx 1, \quad \frac{|\rho(x)|}{N_A} \approx 1.
\]  
(11)

In the quasi-neutral region (outside the SCR), \(\rho(x) \approx 0\).

In the case of the symmetric \(n-p\) junction, the boundary of the SCR can be considered as abrupt at \(N_D = N_A = 10^{19} \text{ cm}^{-3}\), \(N_D = N_A = 10^{18} \text{ cm}^{-3}\). The distribution of electrons and holes has a significant effect on the shape of the SCR boundary (figure 2) at \(N_D = N_A = 10^{17} \text{ cm}^{-3}\), \(N_D = N_A = 10^{16} \text{ cm}^{-3}\). The size of the region in which the equalities (11) are satisfied turns out to be much smaller than the size of the SCR.
Figure 2. Distribution of normalized charge density in the SCR of an abrupt and symmetric n-p junction. 1: $N_D = N_A = 10^{19}$ cm$^{-3}$; 2: $N_D = N_A = 10^{18}$ cm$^{-3}$; 3: $N_D = N_A = 10^{17}$ cm$^{-3}$; 4: $N_D = N_A = 10^{16}$ cm$^{-3}$.

Figure 3. Distribution of normalized charge density in the SCR of an abrupt, asymmetric n-p junction: 1: $N_D = 10^{19}$ cm$^{-3}$, $N_A = 10^{18}$ cm$^{-3}$; 2: $N_D = 10^{19}$ cm$^{-3}$, $N_A = 10^{17}$ cm$^{-3}$; 3: $N_D = 10^{19}$ cm$^{-3}$, $N_A = 10^{16}$ cm$^{-3}$.

In the case of the abrupt asymmetric n-p junction, new regularities arise in the distribution of the charge density (figure 3). In the SCR, a region enriched with charge carriers (electrons) appears, where:
\[ n \geq N_d, \quad \left| \frac{\rho(x)}{N_A} \right| \geq 2. \]  

(12)

At the boundary \( x = +0 \), the following values of the ratio \( \frac{\rho(+0)}{N_A} \) were obtained: 1.12 at \( N_d = 10^{18} \) cm\(^{-3} \); 26.9 at \( N_d = 10^{17} \) cm\(^{-3} \); 357 at \( N_d = 10^{16} \) cm\(^{-3} \); for each of these \( N_d \) values, the size of the enriched region \( d_r \) is 0; 5 nm; 23 nm, respectively.

At \( d_r < x < d_p \), a region depleted of charge carriers is located. The concentration of holes increases with \( x \to d_p \) (the region of charge density gradual change), followed by a quasi-neutral region at \( d_p \leq x \).

In the depletion region, at \( x < 0 \), the electron concentration is \( n < N_D \), but is not negligible, which influences the size of the SCR.

A part of a low-conductivity SCR, in which \( n, p \ll N_A \), exists only in a layer with a lower impurity concentration \( N_A \ll N_D \).

The mentioned regularities determine a significant difference in the properties of a symmetric and asymmetric abrupt \( n-p \) junctions.

4. Conclusion

Numerical modelling of the charge density distribution in \( n-p \) junction shows that the region enriched with charge carriers is formed in the SCR of an equilibrium strongly asymmetric \( n-p \) junction both for the diffusion and abrupt distribution of ionized impurities. Thus, the SCR of the strongly asymmetric \( n-p \) junction contains the following parts: 1st is the highly doped region in which the majority charge carriers partially compensate for the charge of ionized impurities; 2nd is the low-doped region containing ionized impurities of the opposite sign with respect to the first, enriched with charge carriers, increasing the charge of ionized impurities; 3rd is the low-doped region depleted of electrons and holes, containing the charge density created by ionized impurities; 4th is the low-doped region in which the majority charge carriers partially compensate for the charge of ionized impurities.

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