Theory of Nanowire Radial p-n-Junction

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Abstract—We have developed an analytic model for the radial p-n-junction in a nanowire (NW) core-shell structure utilizing as a new building block in different semiconductor devices. The potential distribution through the p-n-junction is calculated and the analytical expressions are derived to compute the depletion region widths. We show that the widths of space charge layers, surrounding the core, are the functions of core radius, which is the manifestation of so called classical size effect. The relationship between the depletion layer width and the built-in potential in the asymptotes of infinitely large core radius transforms to square-root dependence specific for conventional planar p-n-junctions. The explicit equation is derived to compute the capacitance of radial p-n-junction. The current-voltage behavior is also carefully determined taking into account the “short base” effects.

Keyword—Snanowire, p-n- junction, barrier capacitance, high injection.

I. INTRODUCTION

The semiconductor nanowires have the potential to impact many different technologies either through the improved material parameters or by offering a new geometry not possible with bulk or thin film structures. Modern advances in nanotechnology allow to incorporate several material layers with the same or different type of conductivity into a single nanowire (nanorod). Coaxial core/shell nanowire (NW) structures with built-in radial p-n-junctions recently have been reported [1]. This new type of structures represents an important class of nanoscale building blocks with potential for exploring new device concepts, e.g., for photovoltaic applications [2]-[4] or field-effect transistors [5]. The array of NWs in which each wire has a p-n-junction in the radial direction may provide an interesting application in the third generation solar cells technology [6], [7]. The advantage of such solar cells is that the directions of light absorption and carrier collection can be orthogonal, which allows to provide efficient carrier separation in the radial direction for the optically thick NW arrays, even when the minority carrier diffusion lengths are shorter than the optical absorption length.

Therefore it is important issue to develop the theoretical model of the nanowire radial p-n-junctions, hence the good understanding of the device performance will guide designer to choose the best components for optimization. The model for the NW radial p-n-junction will be constructed by extending the analyses of the conventional planar p-n-junction geometry [8] to a cylindrical geometry, taking into account that a considerable portion of core and (or) shell can be covered by space charge and the core radius (shell thickness) can be less or comparable to the diffusion length of minority carriers. The analytical relationships for the depletion region widths versus applied voltage, the maximum electric field across the junction, the capacitance-voltage and the current-voltage characteristics are presented and analyzed as functions of material properties and radius of NW.

II. ELECTROSTATIC CHARACTERISTICS OF RADIAL P-N-JUNCTION

We have focused on NW p-n coaxial homo-junction, consisting of a p-type inner “core” with acceptor concentration \( N_A \) and radius \( R_1 \), capped by n-type outer “shell” with donor concentration \( N_D \) and thickness \( (R_2 - R_1) \). The considered structure is illustrated in Fig. 1 (a).

Considering relatively thick NWs, with a diameter of several 100 nm, we neglect the quantum size effects. The p-n-junction in NW is assumed to be abrupt and the depletion approximation is assumed to be valid. In Fig. 1 (b) the \( r \) axis shows the schematic division of the structure into four regions: the quasi-neutral part of the p-core \( (r \leq R_1 - w_p) \), the depletion part of the p-core (of width \( w_p \) ), the depletion part of the n-shell (of width \( w_n \) ) and the quasi-neutral part of the n-shell \( (r \leq R_2 - R_1 - w_n) \). If the temperature is sufficiently high and all impurities are ionized, the majority charge carriers in the core and shell quasi-neutral regions are: \( p_p = N_A \) for \( R_1 - w_p \leq r \leq R_1 \) and \( n_n = N_D \) for \( R_1 + w_n \leq r \leq R_2 \).

A. Potential Distribution and Depletion Region Width

When p-n-junction is formed along core/shell interface, a fraction of the electrons pass from the n region into the p region, while the holes, on the contrary, pass from the p region into the n region. The space-charge layers are created on both sides of the core/shell interface and potential energy barrier is established, (see Fig. 1 (b)). The electric field arises across the junction and the energy bands bend until the establishment of equilibrium state and the alignment of Fermi energy levels (see Fig. 2 (c)). The “built-in” potential energy barrier that forms along the p-n-junction and has the height defined by work function difference of the core and shell, can be written as usual:
To determine the potential distribution across the junction, we should solve the Poisson equation in cylindrical coordinates.

\[
\frac{1}{r} \frac{d}{dr} \left( r \frac{d\Phi}{dr} \right) = \begin{cases} \frac{e^2 p_p}{\varepsilon_0}, & R_1 - w_p \leq r \leq R_1 \\ \frac{e^2 n_n}{\varepsilon_0}, & R_1 \leq r \leq R_1 + w_n \end{cases}
\]  

(3)

where \( \Phi \) is the potential energy of electrons, \( \varepsilon \) is the permittivity of the semiconductor, \( \varepsilon_0 \) is the electric constant. The potential reference is chosen at the border of depletion region in the p-type core. Thus the boundary conditions at \( r = R_1 - w_p \) and \( r = R_1 + w_n \) present the variation of potential energy across the junction and the requirement that the radial component of the electric field should be zero outside the space charge region:

\[
\Phi (R_1 - w_p) = 0, \quad \frac{d\Phi}{dr} \bigg|_{r=R_1-w_p} = 0
\]  

(4)

\[
\Phi (R_1 + w_n) = -\Phi_w, \quad \frac{d\Phi}{dr} \bigg|_{r=R_1+w_n} = 0.
\]  

(5)

It is easy to see that the solution for (3)-(5) has the form

\[
\Phi (r) = -\frac{e^2 p_p}{4\varepsilon \varepsilon_0} \left[ r^2 - (R_1 - w_p)^2 - 2(R_1 - w_p)^2 \ln \frac{r}{R_1 - w_p} \right] + \ln \frac{r - w_p}{R_1 - w_p}.
\]  

for \( R_1 - w_p \leq r \leq R_1 \).

and

\[
\Phi (r) = -\Phi_w + \frac{e^2 n_n}{4\varepsilon \varepsilon_0} \left[ r^2 - (R_1 + w_n)^2 - 2(R_1 + w_n)^2 \ln \frac{r}{R_1 + w_n} \right] + \ln \frac{r - w_n}{R_1 + w_n},
\]  

(6)

for \( R_1 \leq r \leq R_1 + w_n \).

In our model we ignore the charge on the core/shell interface states, so the electric field continuity at \( r = R_1 \) gives

\[
n_n R_1^2 - (R_1 + w_p)^2 = p_p (R_1 - w_p)^2 - R_1^2
\]  

(7)

which represents the charge neutrality of the junction. Using (6), (7) and demanding the continuity of the potential at the homo-junction interface \( r = R_1 \) we get the following equation for \( w_p \)

\[
\frac{(n_n + p_p) - (1 - w_p)^2}{p_p} \cdot \ln \left( \frac{n_n + p_p}{n_n} - \frac{p_p}{n_n} (1 - w_p) \right)^2 + \left( 1 - w_p \right)^2 \ln \left( 1 - \frac{w_p}{R_1} \right)^2 = -\frac{4\varepsilon \varepsilon_0}{e^2 p_p R_1^2} \Phi_0.
\]  

(8)

Thus for the given \( n_n, p_p, \Phi_w \) and \( R_1 \), the depletion layer widths in the core \( (w_p) \) and in the shell \( (w_n) \) can be calculated from (7), (8).

\[
\Phi_0 = kT \ln \frac{n_n p_p}{n_i^2},
\]  

(1)

where \( kT \) is the thermal energy, \( n_i \) is the intrinsic carrier concentration of the semiconductor. This potential barrier opposes to electron diffusion from the n-type shell to the core and to hole diffusion from the core to the shell, such as the total electron current and the total hole current are both zero at thermal equilibrium.

Close to the junction the concentration of mobile charge sharply decreases and the space charge is mainly formed by ionized donors and acceptors. In complete-depletion approximation the space charge density is:

\[
\rho = \begin{cases} -eN_A = -e \cdot p_p, & R_1 - w_p \leq r \leq R_1 \\ eN_D = e \cdot n_n, & R_1 \leq r \leq R_1 + w_n \end{cases}
\]  

(2)

where \( e \) is the electronic charge.

Fig. 1 Cross section of core/shell NW (a), profile of potential energy across the junction (b), energy band diagram (c)
It is worth to note that in the radial p-n-junction the width of space charge layer is a function of core radius, which is the manifestation of the classical size effect. This means that for the NWs with the same doping level but different radius the depletion layer has different width. For sufficiently large NW radius, when $R_1 \gg w_p$, we compute from (8) the standard relationship for depletion width, which varies with $\Phi_o$ by the square root law as in conventional p-n-junctions: $w_p = \sqrt{\frac{2\varepsilon_0 \varepsilon R_1}{\varepsilon P_p}}$. As it follows from (7) the ratio $w_p/w_n$ depends not only from the doping concentrations but also on NW radius:

$$w_p = \frac{n_p^{2+}n_n^{1+}}{n_p^{2}−w_n} \quad \text{(9)}$$

It is evident from (9) that at equal core and shell doping levels ($n_p = p_p$) the depletion width in the core is always larger than in the shell. This is a specific feature of radial p-n-junctions, whereas in planar geometry at equal donor and acceptor concentrations the junction is symmetric ($w_p = w_n$). In the NW p-n-junctions the widths of depletion layers are limited by the core radius: $w_p < R_1$ and by the shell thickness: $w_n < R_2 - R_1$.

To find $w_p$, $w_n$ under the external bias ($V$), we should replace the built-in energy barrier $\Phi_o$ with $(\Phi_o - eV)$ in the right hand side of (7), and (8), where $V > 0$ means p-core is positively biased with respect to the n-shell. Let us define the critical value of reverse bias ($V_c$), when the nanowire core is totally depleted of holes. By substituting $w_p = R_1$ in (8) we get:

$$\frac{\varepsilon V_c}{\Phi_o} = \frac{\varepsilon^2 n_p + P_p R_1^2}{4\varepsilon_0 \Phi_o} \ln \frac{n_p + P_p}{n_n} - 1 \quad \text{(10)}$$

However, even in the absence of external bias for a given core radius $R_1$ there is a certain ratio of doping concentrations $n_p$ and $p_p$ and, hence, a certain built-in potential barrier $\Phi_o c$ at which the NW core is totally covered by the space charge. From (8) we get:

$$\Phi_o c = \frac{\varepsilon^2 (n_p + p_p) R_1^2}{4\varepsilon_0} \ln \frac{n_p + p_p}{n_n} \quad \text{(11)}$$

Fig. 2 presents the depletion width in the NW core at different core radiuses as a function of applied voltage. It is seen that for a given value of applied voltage, the width of depletion region is smaller for larger radiuses $R_1$ and for sufficiently thick NW it tends to the square root dependence on applied voltages, which is depicted in Fig. 2 by dashed line.

For sufficiently long NW the junction electric field has only radial component and its distribution across the space charge region is different from that in the conventional p-n-junction. In general, it may be expressed by the sum of linear and hyperbolic terms as:

$$E(r) = \frac{\varepsilon P_p (r - (R_1 - w_p)^2)}{2\varepsilon_0 r} \quad \text{if} \quad R_1 - w_p \leq r \leq R_1$$

The maximum of electric field falls at core/shell interface ($r = R_1$) and is given as

$$E_m = \frac{\varepsilon P_p}{2\varepsilon_0} \left(1 + \frac{w_n}{2R_1}\right) = \frac{\varepsilon P_p}{2\varepsilon_0} \left(1 - \frac{w_p}{2R_1}\right) \quad \text{(13)}$$

Thus the maximum value of the electric field depends not only on the doping concentrations and applied voltage but also on NW radius.

**B. Symmetric Radial p-n-Junction**

To form the symmetric p-n-junction, such that $w_p = w_n$, at a given radius $R_1$, the proper ratio of doping concentrations $y = \frac{n_p}{p_p}$ should be chosen. It is evident from (7) that it is possible to have the symmetric radial p-n junction if $y \geq 1$, (i.e. the core should be more heavily doped than the shell).

From (7) and (8) we get the equation for $y$:

$$\frac{1}{y} \left(\ln \frac{3y-1}{y+1}\right)^2 + \left(\ln \frac{3y-1}{y+1}\right)^2 \ln \left(\frac{3y}{y+1}\right) = A \left(\ln \left(\frac{2}{n_n}\right) - \ln(y)\right) \quad \text{(14)}$$
The relationship (17) makes evident that the specific capacitance of radial p-n-junction at \( R_1 \to \infty \), coincides with that for planar p-n-junction. When \( w_p < n_a \) we calculate from (16):

\[
\frac{C}{2\pi L} \approx \frac{-\varepsilon_0}{w_p + w_n} \left( 1 - \frac{w_p}{R_1} \right)^2 \frac{1}{1 + \frac{p_p}{n_n} \left( 1 - \frac{p_p}{n_n} \right)^2} 
\]

where \( w_n \approx w_p \cdot p_p / n_n \).

The relationship (17) makes evident that the specific capacitance of radial p-n-junction at doping concentrations \( p_p < n_a \) is smaller than that of corresponding planar junction, and vice versa at \( p_p > n_n \). Close to the critical value of reverse bias, \( w_p \approx R_1 \), as following from (16), the barrier capacitance of the radial p-n-junction tends to zero in analogy with cylindrical capacitor, when a decrease of the inner plate radius leads to the logarithmical decrease of capacitance \( C = \varepsilon_0 \epsilon \pi L \ln \left( R_2 / R_1 \right) \).

It is seen from (16) that the capacitance of nanowire radial p-n-junction per unit length is determined by the fundamental constant \( \varepsilon_0 (F/m) \). Thus for the NW with \( L = 10 \mu m \) length the junction capacitance is order of 1 to 10 fF.

The Fig. 4 presents the dependence of \( 1/C^2 \) on applied voltage for the NWs with different core diameter.

We verify that the expression for specific capacitance of radial p-n junction at \( R_1 \to \infty \), coincides with that for planar p-n-junction. When \( w_p < n_a \) we calculate from (16):

\[
\frac{C}{2\pi L} \approx \frac{-\varepsilon_0}{w_p + w_n} \left( 1 - \frac{w_p}{R_1} \right)^2 \frac{1}{1 + \frac{p_p}{n_n} \left( 1 - \frac{p_p}{n_n} \right)^2} 
\]
of the shell, without significant recombination in the volume. Consequently, the conditions of the current passage through the shell/metal interface plays important role in the current characteristics. In our analyzes we will follow the standard current transport model of planar short-base diode [7]. We will consider an ideal (ohmic) metallic contact, wrapping the shell, such that the built-in potential barrier, possibly formed at the metal and shell contact, in both accumulation or depletion modes is not higher than several $kT$.

Under these conditions we can write [7]:

$$p(R_2) - p_n = \Delta p(R_2) = 0, \quad n(R_2) = n_m$$  \hspace{1cm} (18)

where $p(R_2)$ and $n(R_2)$ are, respectively, the concentrations of holes and electrons at the surface of the shell, $p_n$ is the minority carrier concentration in the volume of the $n$-shell.

If $d \ll L_n$ then (18) means that the holes injected from the $p$-junction do not accumulate at the semiconductor-metal interface and freely pass to the metal, recombining there with electrons. Therefore the hole recombination process in $n$-region can be ignored. So the net electron and hole currents remain constant throughout the $n$-region:

$$I_p = 2\pi r R D_n \frac{e}{kT} \left( E(r) \cdot r \frac{dp(r)}{dr} \right) = \text{const}$$  \hspace{1cm} (19)

$$I_n = 2\pi r R D_n \frac{e}{kT} \left( E(r) \cdot r \frac{dn(r)}{dr} \right) = \text{const}$$  \hspace{1cm} (20)

where $D_n$ and $D_p$ are the diffusion constants of electrons and holes respectively. $E(r)$ is the radial component of electric field.

In this case, when the carrier recombination does not take place in the shell, the current density passing through the metal-semiconductor contact is $\frac{R_n}{R_1}$ times less than the one crossing the core/shell interface. From other side, it is known that for the same value of applied voltage and for not very large built-in potential barrier, the density of the current passing through the semiconductor/metal contact is much higher than that through the $p$-$n$-junction. In the radial $p$-$n$-junction, as we mentioned, the density of the current through the metallic contact is only $\frac{R_n}{R_1}$ times less than through the $p$-$n$-junction, thus the main potential drop occurs along the $p$-$n$-junction:

$$\Delta p(R_1 + w_n) = p_n \left(e^{\frac{eV}{kT}} - 1\right)$$  \hspace{1cm} (21)

The minority carriers injected into the $n$-shell will induce the redistribution of majority carriers, so that they will quickly compensate the charge of minority carriers resulting in an increase of electron concentration on the same value: $\Delta n(R) = n_n = p(R) - p_n = \Delta p(r)$. Depending on injection level the concentration of non-equilibrium charge carriers at the depletion layer edge in the $n$-region can be comparable to $n_n$ or even higher, i.e.

$$\Delta n(R_1 + w_n) = n_n + \Delta p(R_1 + w_n)$$  \hspace{1cm} (22)

therefore the concentration of injected electrons at the end of depletion layer in the $p$-core should be:

$$\Delta n(R_1 - w_p) = n_p \left[1 + \frac{\Delta p(R_1 + w_n)}{n_n}\left(e^{\frac{eV}{kT}} - 1\right)\right]$$  \hspace{1cm} (23)

It should be noted that by writing the boundary condition for the injected holes in the form of (21) we have assumed that $\Delta n(R_1 - w_p) \ll p_p$. I.e. in the presence of external voltage the height of junction potential barrier still remains larger than $kT$: $\phi_n - eV_i \gg kT$. In such conditions, when $p_p \gg n_m$ the electron current $(I_n)$ through the $p$-n junction is very small compared with the hole current $(I_p)$.

As the bulk recombination is assumed to be very small, we can consider $I_n \approx 0$, then it is easy to find the radial component of electric field in the $n$-region:

$$E(r) \approx -\frac{kT}{e} \frac{dn}{dr}.$$  \hspace{1cm} (24)

By substituting (24) into (19) and by taking into account the quasi-neutrality of $n$-region we can express the net hole current as:

$$I_p = -2\pi r R D_n \left(2 - \frac{n_n}{n_n + \Delta p(r)}\right) \frac{dp(r)}{dr}.$$  \hspace{1cm} (25)

Then multiplying (25) by $r^{-1}$ and by integrating it between $(R_1 + w_n)$ and $R_Z$ for $I_p = \text{const}$ we get:

$$I_p = \frac{2\pi e D_n p_n}{\ln(\frac{R_Z}{R_1 + w_n})} \left(\frac{2}{\frac{n_n}{n_p}} \ln \left[1 - \frac{p_p}{n_n} \left(e^{\frac{eV}{kT}} - 1\right)\right]\right) - \frac{2}{\frac{n_n}{n_p}} \ln \left[1 - \frac{p_p}{n_n} \left(e^{\frac{eV}{kT}} - 1\right)\right].$$  \hspace{1cm} (26)

Using the boundary conditions (18) and (22) we can find the potential drop in quasi-neutral part of the shell:

$$V_2 = \int_{R_1 + w_n}^{R_2 + w_d} E \, dr = \frac{kT}{e} \ln \left[1 - \frac{n_n}{n_p} \left(e^{\frac{eV}{kT}} - 1\right)\right].$$  \hspace{1cm} (27)

Thus for the given applied voltage $V = V_1 + V_2$ by using the relationship (27) we can define the voltage drops on p-n junction and on its base (shell).

At first we consider the case of small applied voltages corresponding to the weak injection regime of holes, when $\Delta p(R_1 + w_n) \ll n_m$. As it follows from (27) the voltage drop in the shell is very small: $eV_2 \ll kT$, and $V_1 \approx V$ so for the junction current we have:

$$I_p = \frac{2\pi e D_n p_n}{\ln(\frac{R_Z}{R_1 + w_n})} \left(e^{\frac{eV}{kT}} - 1\right).$$  \hspace{1cm} (28)

It is seen from the last relationship, that at small forward bias the current increases as $e^{\frac{eV}{kT}}$. In this case the concentration of non-equilibrium charge carriers decreases in n-region very
slowly: logarithmically, and not linearly as in conventional planar junctions,

$$\Delta p(r) = \Delta p(R_1 + w_n) \frac{ln \frac{R_2}{R_1}}{ln \frac{R_2}{R_1 + w_n}} \quad (29)$$

Therefore, as it follows from (28) the magnitude of junction net current is defined by the value of $2\pi l (R_1 + w_n) \frac{d\Delta p}{dr}$ at the edge of depletion layer, which is:

$$\frac{d\Delta p(R_1 + w_n)}{dr} = - \frac{\Delta p(R_1 + w_n)}{(R_1 + w_n) ln \frac{R_2}{R_1 + w_n}} \quad (30)$$

The depletion width $w_n$ increases at high reverse biases and therefore the width of quasi-neutral part of the shell decreases, then, due to the increase of the hole concentration gradient the junction current, according to (28), continues to slowly increase instead to become saturated, which is a specific feature of devices with planar geometry and thick base.

The situation with current transport is quite different when high forwarding bias is applied and the minority carrier injection is enhanced, such that, $p' (R_1 + w_n) \gg n_n$ or $eV_1 \gg kT \ln \frac{n_n}{n_i}$. Then from (27) it follows that the voltage drops on the shell volume and on the junction are:

$$V_2 = V_1 = \frac{kT}{e} \ln \frac{n_n}{n_i} = \frac{V}{2} = \frac{kT}{e} \ln \frac{n_n}{n_i} \quad (31)$$

Substituting $V_1$ into the (26) for the current we can write

$$I_p \approx \frac{2\pi e D_p \frac{n_n}{2}}{ln (R_2 / R_1 + w_n)} exp \left( \frac{eV}{2kT} \right) \quad (32)$$

Thus, if an applied voltage is in the range: $\frac{2kT}{e} \ln \frac{n_n}{n_i} < V < 2\frac{kT}{e} \ln \frac{P_n}{n_i}$, the main part of the voltage drop occurs on the quasi-neutral region of n-shell and the junction current starts to increase less sharply, proportional to $exp \left( \frac{eV}{2kT} \right)$.

Such behavior of the current-voltage characteristics is illustrated in Fig. 5. The calculations are done by solving (26) and (27) and the results are shown in linear and logarithmic scales. It is seen, that the slope of $ln(I/I_0)$, where $I_0 = 2pe D_p \frac{n_n}{L} l_e$ decreases almost two times with an increase of applied voltage, which means that the forward current of the NW radial p-n-junction starts to increase with significantly reduced slope at high applied voltages. Such specific feature of current-voltage characteristics was observed experimentally for gallium arsenide NW radial p-n-junctions [4].

**Fig. 5** The current versus applied forward bias in linear scale (right axes) and in logarithmic scale (left axes)

It should be noted that even at high injection level the distribution of non-equilibrium charge carriers stays logarithmical along the NW’s radius. Indeed, for $\Delta p(r) \gg n_n$ it follows from (25)

$$I_p \approx -2eD_p \left(2\pi r L \frac{dp}{dr} \right) = const.$$  \quad (33)

i.e. the hole ohmic current is exactly equal to the diffusion current, and their distribution is described by the relationship (29).

**V. CONCLUSION**

The theoretical analysis is performed for the radial p-n-junction. The final sizes of the NW core and shell are accounted in the model. The analytical expressions are derived to calculate the widths of depletion layers, the barrier capacitance and the volt-ampere characteristics. The developed model is a good base for further studies of built-in junctions in the core/shell NWs, particularly its photovoltaic applications.

**REFERENCES**


