Best Performance of $n^+ - p$ Crystalline Silicon Junction Solar Cells at 300 K, Due to the Effects of Heavy Doping and Impurity Size. I

Huynh Van Cong*, Paul Blaise*, Olivier Henri-Rousseau

Department of Physics, Laboratory of Mathematics and Physics, University of Perpignan, Perpignan, France

Email address: huynh@univ-perp.fr (H. V. Cong), huynhvc@outlook.fr (H. V. Cong), blaise@univ-perp.fr (P. Blaise)

*Corresponding author

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Abstract: The effects of heavy doping and donor (acceptor) size on the hole (electron)-minority saturation current density $J_{Eo}(J_{Bo})$, injected respectively into the heavily (lightly) doped crystalline silicon (Si) emitter (base) region of $n^+ - p$ junction, which can be applied to determine the performance of solar cells, being strongly affected by the dark saturation current density: $J_o \equiv J_{Eo} + J_{Bo}$, were investigated. For that, we used an effective Gaussian donor-density profile to determine $J_{Eo}$, and an empirical method of two points to investigate the ideality factor $n$, short circuit current density $J_{sc}$, fill factor (FF), and photovoltaic conversion efficiency $\eta$, expressed as functions of the open circuit voltage $V_{oc}$, giving rise to a satisfactory description of our obtained results, being compared also with other existing theoretical-and-experimental ones. So, in the completely transparent and heavily doped (P-Si) emitter region, CTHD(P-Si)ER, our obtained $J_{Eo}$-results were accurate within 1.78%. This accurate expression for $J_{Eo}$ is thus imperative for continuing the performance improvement of solar cell systems. For example, in the physical conditions (PCs) of CTHD (P-Si) ER and of lightly doped (B-Si) base region, LD(B-Si)BR, we obtained the precisions of the order of 8.1% for $J_{sc}$, 7.1% for FF, and 5% for $\eta$, suggesting thus an accuracy of $J_{Bo}$ (≤ 8.1%). Further, in the PCs of completely opaque and heavily doped (S-Si) emitter region, COHD(S-Si)ER, and of lightly doped (acceptor-Si) base region, LD(acceptor-Si)BR, our limiting $\eta$-results are equal to: 27.77%, ..., 31.55%, according to the $E_{gi}$-values equal to: 1.12eV, ..., 1.34eV, given in various (B, ..., Tl)-Si base regions, respectively, being due to the acceptor-size effect. Furthermore, in the PCs of CTHD (donor-Si) ER and of LD(Tl-Si)BR, our maximal $\eta$-values are equal to: 24.28%, ..., 31.51%, according to the $E_{gi}$-values equal to: 1.11eV, ..., 1.70eV, given in various (Sb, ..., S)-Si emitter regions, respectively, being due to the donor-size effect. It should be noted that these obtained highest $\eta$-values are found to be almost equal, as: 31.51% ≈ 31.55%, coming from the fact that the two obtained limiting $J_{Eo}$-values are almost the same.

Keywords: Donor (Acceptor)-Size Effect, Heavily Doped Emitter Region, Ideality Factor, Open Circuit Voltage, Photovoltaic Conversion Efficiency

1. Introduction

The minority-carrier transport in the non-uniformly and heavily doped (NUHD), quasi-neutral, and uncompensated emitter region of impurity-silicon (Si) devices such as solar cells and bipolar transistors at temperature $T(= 300 \text{ K})$, plays an important role in determining the behavior of many semiconductor devices [1-29]. It should be noted that the minority-carrier saturation current density, $J_{Eo}$, injected into this emitter region strongly controls the common emitter current gain [4-8]. Thus, an accurate determination of this $J_{Eo}$ or an understanding of minority-carrier physics inside heavily doped semiconductors is imperative for continuing the performance improvement of bipolar transistors, and that of solar cell systems, which is commonly characterized in terms of the parameters such as: the ideality factor $n$, short circuit current density $J_{sc}$, fill factor FF, and photovoltaic conversion efficiency $\eta$, being
expressed as functions of the open circuit voltage $V_{oc}$.[4]

Further, it should be noted that, in most fabricated silicon devices, the effective Gaussian donor-density profile $\rho(x)$, being proposed in next Equation (24), varies with carrier position $x$ in the emitter region of width $W$ [13, 18-20, 22], and it decreases with increasing $W$, being found to be in good agreement with that used by Essa et al. [13]. As a result, many other physical quantities, given in this NUHD emitter region of minority-hole (electron) diffusion length $L_{h(e)}$, minority-hole (electron) mobility $\mu_{h(e)}$, minority-hole (electron) lifetime $\tau_{h(e)}$, and minority-hole (electron) diffusion length $L_{h(e)}$, strongly depend on $\rho(x)$.

In the present paper, we determine an accurate expression for the minority-hole current density $J_{eo}$, injected into the NUHD emitter region of $n^+ - p$ junction silicon solar cells at 300 K, being also applied to determine the performance of such crystalline silicon solar cells.

In Section 2, we study the effects of impurity size [or compression (dilation)], temperature and heavy doping, affecting the energy-band-structure parameters such as: the intrinsic band gap $E_{Gi}$, intrinsic carrier concentration $n_i$, band gap narrowing $\Delta E_g$, Fermi energy $E_F$, apparent band gap narrowing $\Delta E_{ga}$, and effective intrinsic carrier concentration $n_\epsilon$. In Section 3, an accurate expression for the optical band gap (OBG), $E_{Gi}$, is investigated in next Equation (16), being accurate within 1.86%, as showed in Table 3. Some useful minority-carrier transport parameters such as: $\mu_h$ and $L_h$, being given in the heavily doped $n$-type emitter region, and $\mu_e$, $\tau_e$ and the minority-electron saturation current density $J_{Bo}$, being given in the lightly doped $p$-type base region, are also presented in Section 4. Then, in Section 5, an accurate expression for the minority-hole saturation current density $J_{eo}$, injected into the heavily doped emitter region of $n^+ - p$ junction silicon solar cells at 300 K is established in Equation (39) or its approximate form given in Eq. (44), indicating an accuracy of the order of 1.78%, as seen in Table 4. Further, the total saturation current density: $J_0 = J_{eo} + J_{Bo}$, where $J_{Bo}$ [1, 7], determined in Equation (21), is the minority-electron saturation current density $J_{Bo}$, injected into the lightly doped base region of $n^+ - p$ junction silicon solar cells, can be used to investigate the photovoltaic conversion effect, as presented in Section 6. Finally, some concluding remarks are given and discussed in Section 7.

### 2. Energy-Band-Structure Parameters in Donor (Acceptor)-Si Systems

Here, we study the effects of donor (acceptor) [d(a)]-size, temperature, and heavy doping on the energy-band-structure parameters of $d(a)$-Si systems, as follows.

#### 2.1. Effect of $d(a)$-Size

In $d(a)$-Si-systems at T=0 K, since the $d(a)$-radius $r_{d(a)}$, in tetrahedral covalent bonds is usually either larger or smaller than the Si atom-radius $r_0$, assuming that in the P(B)-Si system $r_{P(B)} = r_0 = 0.117 nm$, with $1 nm = 10^{-8}m$, a local mechanical strain (or deformation potential energy) is induced, according to a compression (dilation) for $r_{d(a)} < r_0$ ($r_{d(a)} < r_0$), respectively, due to the $d(a)$-size effect. Then, in the Appendix A of our recent paper [42], basing on an effective Bohr model, such a compression (dilation) occurring in various $d(a)$-Si systems was investigated, suggesting that the effective dielectric constant, $\varepsilon(r_{d(a)})$, decreases with increasing $r_{d(a)}$. This $r_{d(a)}$-effect thus affects the changes in all the energy-band-structure parameters, expressed in terms of $\varepsilon(r_{d(a)})$, noting that in the P(B)-Si system $\varepsilon(r_{P(B)}) = 11.4$. In particular, the changes in the unperturbed intrinsic band gap, $E_{geo}(r_{P(B)}) = 1.17 eV$, and effective $d(a)$-ionization energy in absolute values $E_{d(a)}(r_{P(B)}) = 33.58 meV$, are obtained in an effective Bohr model, as [42]:

$$E_{geo}(r_{d(a)}) - E_{geo}(r_{P(B)}) = E_{d(a)}(r_{d(a)}) - E_{d(a)}(r_{P(B)}) = E_{d(a)}(r_{P(B)}) \times \left[ \frac{\varepsilon(r_{P(B)})}{\varepsilon(r_{d(a)})} \right]^2 - 1 \quad (1)$$

Therefore, with increasing $r_{d(a)}$, the effective dielectric constant $\varepsilon(r_{d(a)})$ decreases, implying that $E_{geo}(r_{d(a)})$ increase. Those changes, which were investigated in our previous paper [42], are now reported in the following Table 1, in which the data of the critical $d(a)$-density $N_{cn}\varepsilon_{(d(a))}$ are also reported. This critical density marks the metal-to-insulator transition from the localized side (all the impurities are electrical neutral), $N(N_d) \leq N_{cn}\varepsilon_{(d(a))}$, to the extended side, $N(N_d) \geq N_{cn}\varepsilon_{(d(a))}$, assuming that all the impurities are ionized even at 0 K. However, at $T = 300 K$, for example, all the impurities are thus ionized and the physical conditions, defined by: $N(N_d) > N_{cn}\varepsilon_{(d(a))}$ and $N(N_d) < N_{cn}\varepsilon_{(d(a))}$, can thus be used to define the $n(p)$-type heavily and lightly doped Si, respectively.

### Table 1. The values of $r_{d(a)}$, $\varepsilon(r_{d(a)})$, and $E_{geo}(r_{d(a)})$, and critical impurity density $N_{cn}\varepsilon_{(d(a))}$, obtained in our previous paper [42], are reported here.

<table>
<thead>
<tr>
<th>Donor</th>
<th>Sb</th>
<th>P</th>
<th>As</th>
<th>Bi</th>
<th>Ti</th>
<th>Te</th>
<th>Se</th>
<th>S</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T=0 K$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$r_{d}$ (nm)</td>
<td>0.1131</td>
<td>0.1170</td>
<td>0.1277</td>
<td>0.1292</td>
<td>0.1424</td>
<td>0.1546</td>
<td>0.1621</td>
<td>0.1628</td>
</tr>
<tr>
<td>$\varepsilon(r_{d})$</td>
<td>12.02</td>
<td>11.40</td>
<td>8.47</td>
<td>7.95</td>
<td>4.71</td>
<td>3.26</td>
<td>2.71</td>
<td>2.67</td>
</tr>
<tr>
<td>$E_{geo}(r_{d})$(eV)</td>
<td>1.167</td>
<td>1.170</td>
<td>1.197</td>
<td>1.205</td>
<td>1.333</td>
<td>1.547</td>
<td>1.729</td>
<td>1.749</td>
</tr>
<tr>
<td>$N_{d}(r_{d})(10^{18} cm^{-3})$</td>
<td>3</td>
<td>3.52</td>
<td>8.58</td>
<td>10.37</td>
<td>50</td>
<td>150.74</td>
<td>261.24</td>
<td>274.57</td>
</tr>
</tbody>
</table>
2.2. Temperature Effect

Being inspired from excellent works by Pässler [33, 34], who used semi-empirical descriptions of T-dependences of band gap of the Si by taking into account the cumulative effect of electron-phonon interaction and thermal lattice expansion mechanisms or all the contributions of individual lattice oscillations [33-35], we proposed in our recent paper [43] a simple accurate expression for the intrinsic band gap in the silicon (Si), due to the T-dependent carrier-lattice interaction-effect, \( E_{\text{gi}}(T, r_d(a)) \), by

\[
E_{\text{gi}}(T, r_d(a)) = E_{\text{go}}(r_d(a)) - 0.071 \text{ (eV)} \times \left\{ \left[ 1 + \left( \frac{2T}{440.6913K} \right)^2 \right]^{-1} - 1 \right\}
\]

where the values of \( E_{\text{go}}(r_d(a)) \) due to the d(a)-size effect are given in Table 1 and those of \( E_{\text{gi}}(T = 300 \text{ K}, r_d(a)) \) tabulated in Table 2. Further, as noted in this Reference 43, in the (P, S)-Si systems, for 0 K \( \leq T \leq 3500 \text{ K} \), the absolute maximal relative errors of this \( E_{\text{gi}} \)-result were found to be equal respectively to: 0.22% and 0.15%, calculated using the very accurate complicated results given by Pässler [34]. Then, in the n-type HD silicon at temperature T, the effective mass of the majority electron can be defined by [31, 32]:

\[
m_e(T, r_d) = \left[ 0.9163 \times \left( \frac{1.1905 \times E_{\text{go}}(r_d)}{E_{\text{gi}}(T, r_d)} \right) \right]^{2/3} \times m_0 = \frac{m_0}{C/W}
\]

which gives: \( m_{\text{eo}} = m_e(T = 0 \text{ K}) = 0.3216 \times m_0 \), \( m_0 \) being the electron rest mass, and the effective mass of the minority hole yields [31, 32]:

\[
m_v(T) = \frac{2}{3} \left( \frac{0.943587 + 0.369528 \times 10^{-2} + 0.117351 \times 10^{-3} T + 0.126218 \times 10^{-4} T^2 + 0.302551 \times 10^{-5} T^3 + 0.172481 \times 10^{-6} T^4}{1 + 0.468338 \times 10^{-3} + 0.228689 \times 10^{-4} T + 0.746927 \times 10^{-5} T^2 + 0.172748 \times 10^{-6} T^3} \right) \times \frac{m_0}{C/W}
\]

which gives \( m_v(T = 0 \text{ K}) = 0.3664 \times m_0 \). Here, \( g_v = 2 \) is the effective average number of equivalent valence-band edges. Now, the intrinsic carrier concentration \( n_i \) is defined by

\[
n_i(T, r_d(a), g_e) \equiv N_c(T, r_d, g_e) \times N_e(T, g_v) \times \exp \left( \frac{-E_{\text{gi}}(T, r_d(a))}{k_B T} \right)
\]

where, \( N_c(T) \) is the conduction (valence)-band density of states, given by [31, 32]:

\[
N_c(T, r_d, g_e) = 2g_e \times \left( \frac{m_e(T, r_d) \times k_B T}{2\pi \hbar^2} \right)^{3/2} \text{ (cm}^{-3}\text{)} \quad \text{(6)}
\]

\[
N_e(T, g_v) = 2g_v \times \left( \frac{m_v(T, g_v) \times k_B T}{2\pi \hbar^2} \right)^{3/2} \text{ (cm}^{-3}\text{)} \quad \text{(7)}
\]

where \( \hbar = h/2\pi \) is the Dirac’s constant, \( k_B \) is the Boltzmann constant, and \( g_e \) is the effective average number of equivalent conduction-band edges. Moreover, for \( r_d \equiv r_p \) and at 300 K, some typical \( n_i \)-results obtained for different \( g_e \)-values, calculated using Equation (5), are given as follows.

(i) If \( g_e = 6 \), one then obtains: \( n_i = 10.7 \times 10^9 \text{ cm}^{-3} \), being just a result investigated from a measurement of energy-band-structure parameters and intrinsic conductivity by Green [31].

(ii) If \( g_e = 5 \), one then obtains: \( n_i = 9.77 \times 10^9 \text{ cm}^{-3} \), according to a result given from a capacitance measurement of a pin diode biased under high injection, by Misiakos and Tsamakis [37].

(iii) Finally, if \( g_e = 4.9113 \), one then gets: \( n_i = 9.68 \times 10^9 \text{ cm}^{-3} \), according to a result proposed by Coudere et al. (C) as [38]: \( n_i(g_e) = 1.541 \times 10^{15} \times T^{3.721} \times \exp \left( \frac{-E_{\text{gi}}}{k_B T} \right) \text{ cm}^{-3} = 9.68 \times 10^9 \text{ cm}^{-3} \) for \( T = 300 \text{ K} \), basing on their updated fit of experimental data for the minority-carrier mobility and open-circuit voltage decay, which were given by Sproul and Green [36]. Further, from Equations (5, 2), in donor-Si systems and for \( T = 300 \text{ K} \), the numerical results of \( n_i \) and \( E_{\text{gi}} \), calculated for \( g_e = 6, 5, \) and 4.9113, as functions of \( r_d(a) \), are tabulated in Table 2.

### Table 2. The values of intrinsic carrier concentration \( n_i(T = 300 \text{ K}, r_d(a), g_e) \) and intrinsic band gap \( E_{\text{gi}} \) are calculated for \( g_e = 6, 5, \) and 4.9113, using Equations (5, 2), respectively, as functions of \( r_d(a) \).

<table>
<thead>
<tr>
<th>Donor ( g_e )</th>
<th>Sb</th>
<th>P</th>
<th>As</th>
<th>Bi</th>
<th>Ti</th>
<th>Te</th>
<th>Se</th>
<th>S</th>
</tr>
</thead>
<tbody>
<tr>
<td>( g_e = 6 )</td>
<td>0.1125</td>
<td>1.1245</td>
<td>1.1515</td>
<td>1.1595</td>
<td>1.2875</td>
<td>1.5015</td>
<td>1.6835</td>
<td>1.7035</td>
</tr>
<tr>
<td>( E_{\text{gi}}(300 \text{ K}) ) in eV</td>
<td>1.1215</td>
<td>1.07</td>
<td>6.24 \times 10^{-1}</td>
<td>5.43 \times 10^{-1}</td>
<td>4.56 \times 10^{-2}</td>
<td>7.26 \times 10^{-4}</td>
<td>2.14 \times 10^{-5}</td>
<td>1.46 \times 10^{-5}</td>
</tr>
<tr>
<td>( n_i(300 \text{ K}) ) in ( 10^9 \text{ cm}^{-3} )</td>
<td>1.13</td>
<td>1.07</td>
<td>6.24 \times 10^{-1}</td>
<td>5.43 \times 10^{-1}</td>
<td>4.56 \times 10^{-2}</td>
<td>7.26 \times 10^{-4}</td>
<td>2.14 \times 10^{-5}</td>
<td>1.46 \times 10^{-5}</td>
</tr>
</tbody>
</table>
2.3. Heavy Doping Effect

First of all, in the donor-Si system, we define the effective intrinsic carrier concentration \(n_i^2\), by

\[
n_i^2 = N \times p_o \equiv n_i^2 \times \exp\left(\frac{\Delta E_g}{k_B T}\right)
\]

where \(n_i^2\) is determined in Equation (5). Here, we can also define the “effective doping density” by [8]:

\[
N_{\text{eff}} = N_{\text{def}} \equiv N / \exp\left(\frac{\Delta E_g}{k_B T}\right)
\]

so that \(N_{\text{def}} \times p_o = n_i^2\). Here, \(p_o\) is the density of minority holes at the thermal equilibrium and the ABGN is defined by:

\[
\Delta E_{g_{\text{a}(k)}}(N) = 8.5 \times 10^{-3} \times \left[\ln\left(\frac{N}{1.33 \times 10^{10} \text{ cm}^{-3}}\right) + \left[\ln\left(\frac{N}{1.33 \times 10^{10} \text{ cm}^{-3}}\right)\right]^2 + 0.5\right] \text{ (eV)}
\]

\[
\Delta E_{g_{\text{a}(kSG)}}(N) = 6.92 \times 10^{-3} \times \left[\ln\left(\frac{N}{1.33 \times 10^{10} \text{ cm}^{-3}}\right) + \left[\ln\left(\frac{N}{1.33 \times 10^{10} \text{ cm}^{-3}}\right)\right]^2 + 0.5\right] \text{ (eV)}
\]

\[
\Delta E_{g_{\text{a}(ZA)}}(N) = 18.7 \times 10^{-3} \times \ln\left(\frac{N}{7 \times 10^{10} \text{ cm}^{-3}}\right) \text{ (eV)}
\]

\[
\Delta E_{g_{\text{a}(SC)}}(N) = 14 \times 10^{-3} \times \ln\left(\frac{N}{4 \times 10^{10} \text{ cm}^{-3}}\right) \text{ (eV)}
\]

\[
\Delta E_{g_{\text{a}(YC)}}(N) = 4.2 \times 10^{-5} \times \ln\left(\frac{N}{10 \times 10^{10} \text{ cm}^{-3}}\right)^3 \text{ (eV)}
\]

Then, in such the P-Si system at 300K, being inspired by

\[
\Delta E_{g_{\text{a}(\text{Mod.YC})}}(N, g_e) = 114.94 \times 10^{-6} \times \ln\left(\frac{\sqrt{16.747} \times N \times 6}{g_e}\right)^3 \text{ (eV)} = 114.94 \times 10^{-6} \times \ln\left(\frac{N}{3.5 \times 10^{16} \text{ cm}^{-3}}\right)^3 \text{ (eV)}
\]

having a same empirical form as that given in Equation (14).
Figure 2. (c1, c2) our ABGN-results given in heavily doped donor-Si systems, with a condition: $N > N_{ci}(r_d)$.

Now, for $g_c = 6$, in d-Si systems at 300 K, our numerical ABGN ($\Delta E_{ga}$)-results are calculated, using Equation (9). First, ours, obtained for the P-Si system, are plotted as a function of $N$ in Figure 1 (a), in which, for a comparison, the other ones, calculated using Equations (10-15), are also included. Secondly, in this P-Si system, the relative deviations between ours and the others are also plotted as functions of $N$ in Figure 1 (b). Finally, in Figure 2 (c1, c2), ours are plotted in donor-Si systems as functions of $N$.

Here, one observes that:

(i) our numerical ABGN-results obtained using Equations (9, 15) are found to be closed together as seen in Figure 1 (a), and their absolute maximal relative deviation yields: 3.03%, which occurs at $N = 1.2 \times 10^{20}$ cm$^{-3}$, as observed in Figure 1 (b), and

(ii) in Figure 2 (c1, c2), for a given donor-Si system, due to the heavy doping effect, ours increase with increasing $N$, and for a given $N$, ours increase ($\S$) with increasing $r_d^*$, due to the donor-size effect.

Then, in the following, it is possible to define the optical band gap (OBG), expressed in terms of the ABGN (or BGN), suggesting a conjunction between the electrical-and-optical phenomena.

3. Conjunction Between Electrical-and-Optical Phenomena

First of all, we define the optical band gap (OBG) by [25]:

$$E_{g1}(N, T, r_d, g_c) \equiv E_{g1}(T, r_d) - \Delta E_g(N, T, r_d, g_c) + E_F(N, T, r_d, g_c)$$  \hspace{1cm} (16)

where the intrinsic band gap $E_{g1}$ is determined in Equation (2), the BGN $\Delta E_g$ is investigated in Equation (A9) of the Appendix B, and the Fermi energy $E_F$ is given in Equation (A3) of the Appendix A, suggesting that the optical phenomenon is represented by $E_{g1}$. Furthermore, it is possible to establish a conjunction between the electrical and optical phenomena, obtained from Equations (9, 16), as:

$$E_{g1(\text{Mod.YC})}(N, T, r_d, g_c) \equiv E_{g1}(T, r_d) - \Delta E_{ga(\text{Mod.YC})}(N, g_c) + k_B T \times \ln \left( \frac{N}{N_{ci}(T, r_d, g_c)} \right)$$ \hspace{1cm} (17)

Now, in the P-Si system, our numerical OBG-results, calculated using Equations (16, 17) for $g_c = 6, 5, 4.9113$ and at $T=300$ K, are tabulated in following Table 3, in which our numerical results of $E_{g1}^1$ and $E_{g1(\text{Mod.YC})}$, obtained for $g_c = 6$, are accurate within 1.86% and 1.9%, respectively, and found to be the best ones, compared with those obtained for $g_c = 5, 4.9113$. One notes that the relative deviations (RDs) between calculated $E_{g1}$-results and $E_{g1}$-data [44] are defined by: $1 - \frac{\text{Calculated } E_{g1} \text{-results}}{\text{Calculated } E_{g1} \text{-data}}$.}

<table>
<thead>
<tr>
<th>$N$ (10$^{18}$ cm$^{-3}$)</th>
<th>4</th>
<th>8.5</th>
<th>15</th>
<th>50</th>
<th>80</th>
<th>150</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_{g1}$ (eV)-data [44]</td>
<td>1.020</td>
<td>1.028</td>
<td>1.033</td>
<td>1.050</td>
<td>1.056</td>
<td>1.059</td>
</tr>
<tr>
<td>Our OBG-results are obtained, using Equation (16). $g_c = 6$</td>
<td>$E_{g1}$ (eV)</td>
<td>1.0390</td>
<td>1.0465</td>
<td>1.0496</td>
<td>1.0483</td>
<td>1.0463</td>
</tr>
<tr>
<td>RD(%)</td>
<td>-1.86</td>
<td>-1.80</td>
<td>-1.61</td>
<td>0.17</td>
<td>0.92</td>
<td>1.05</td>
</tr>
</tbody>
</table>
4. Minority-Carrier Transport Parameters

Here, in the heavily doped n-type emitter region and the lightly doped p-type base region of n⁺ - p junction silicon solar cells, the minority-hole (electron) transport parameters are studied as follows.

4.1. Heavily Doped n-type Emitter-region Parameters

In order to determine the minority-hole saturation-current density \( J_{60} \), injected into the heavily doped n-type emitter-region, we need to know an expression for the minority-hole mobility \( \mu_h \), being related to the minority-hole diffusion coefficient \( D_h \), by the well-known Einstein relation: \( D_h = \frac{kT}{e} \mu_h \), where \( e \) is the positive hole charge. Here, in donor-Si systems at 300 K and for any \( g_c \), since the minority-hole mobility depends on \( N \) [10], and also on \( g_c \) and \( \varepsilon(r_d) \) [11], we can propose:

\[
\mu_h(N, T, r_d, g_c) = \left[ 130 + \frac{500-130}{1+\frac{1}{10^{g_c} \times \frac{\text{cm}^2}{\text{cm}^3}}} \right] \times \left( \frac{\varepsilon(r_d)}{\varepsilon(r_p)} \right)^2 \times \left( \frac{T}{300 \text{K}} \right)^{3/2} \quad (18)
\]

noting that as \( T = 300 \text{ K} \), \( g_c = 6 \), and \( r_d \equiv r_p \), Equation (18) is reduced to that given by del Alamo et al. [10]. Moreover, Equation (18) indicates that, for a given \( N \) and with increasing \( r_d \), \( \mu_h \) decreases, since \( \varepsilon(r_d) \) decreases as seen in Table 1, being due to the \( d \)-size effect, in good accordance with that observed by Logan et al. [9]. Further, from Equations (5, 8, 9, 15, 18), we can define the following minority-hole transport parameter \( F \) as [22, 25]:

\[
F(N, T, r_d, g_c) \equiv \frac{n_i^2}{p_0 \times D_h} = \frac{N_{\text{Def}}}{D_h \times \exp \left[ \frac{\Delta E}{k_B T} \right]} (\text{cm}^{-5} \times \text{s})
\]

\[
N_{\text{Def}} \equiv \frac{N}{\exp \left[ \frac{\Delta E_{g\text{a}}}{k_B T} \right]} \quad (19)
\]

where \( N_{\text{Def}} \) is the “effective doping density” [8] and the \( \Delta E_{g\text{a}} \) is determined in Equation (9) for our \( \Delta E_{g\text{a}} \)-result or in Equation (15) for our approximate \( \Delta E_{g\text{a}} \)-one.

Furthermore, the minority-hole length, \( L_h(N, T, r_d, g_c) = \frac{\sqrt{\varepsilon(r_d) \times D_h}}{\tau_h} \), \( \tau_h \) being the minority-hole lifetime, can be determined by [22, 25]:

\[
L_h^2(N, T, r_d, g_c) = \left[ \frac{\varepsilon(r_d) \times D_h}{\tau_h} \right]^{-1/2} = \left( C \times F \right)^2 = \left( C \times \frac{N_{\text{Def}}}{D_h} \right)^2 - \left( \frac{C \times \frac{n_i^2}{p_0 \times D_h}}{N} \right)^2 \quad (20)
\]

where the constant \( C = 10^{-17} (\text{cm}^4/\text{s}) \) was chosen in this work. Here, one remarks that \( \tau_h \) can be computed since \( D_h \) (or \( \mu_h \) and \( F \) are determined respectively in Equations (18, 19).

4.2. Lightly Doped p-type Base-Region Parameters

Here, the minority-electron saturation current density injected into the lightly doped p-type base region, with an acceptor density equal to \( N_a \), is given by [1, 7]:

\[
J_{BO}(N_a, T, r_a) = \frac{\varepsilon (N_a, T, r_a)}{N_a} \quad (21)
\]

where \( n_i^2(T, r_d, g_c = 6) \) is determined in Equation (5) and \( D_e(N_a, T, r_a) \equiv \frac{kbT}{e} \mu_e(N_a, T, r_a) \) is the minority-electron diffusion coefficient, noting that Equation (21) is valid only for \( N_a \leq 10^{16} \text{ cm}^{-3} \).

Here, in the acceptor-Si system, \( \mu_e \) is the minority-electron mobility, being determined by [3, 11, 16]:

\[
\mu_e(N_a, T, r_a) = \frac{92 + \frac{1360-92}{1+\frac{1360-92}{10^{8} \text{cm}^{-3}}} \times \left( \frac{\varepsilon(r_a)}{\varepsilon(r_p)} \right)^2 \times \left( \frac{T}{300 \text{K}} \right)^{3/2}}{\text{cm}^2 \text{V}^{-1} \text{s}^{-1}} \quad (22)
\]

being reduced to the result obtained by Slotboom and de Graaff [3, 16], as \( T=300 \text{ K} \) and \( r_a = r_B \), and \( \tau_e(N_a) \) is the
minority-electron lifetime, computed by [16, 25]:
\[ \tau_e(N_d)^{-1} = \frac{1}{2.5 \times 10^{-13}} + 3 \times 10^{-13} \times N_d + 1.83 \times 10^{-31} \times N_d^2. \] (23)

Furthermore, Equation (22) indicates that, for a given \( N_d \) and with increasing \( \tau_e, \mu_h \) decreases, since \( \epsilon(\tau_e) \) decreases, as seen in Table 1, in good accordance with that observed by Logan et al. [9].

Then, in P(B)-Si systems at 300 K and for \( g_c = 6 \), Klaassen et al. confirmed, in Figures 1 and 2 of their paper [16], that the expressions (18, 22) for minority-hole (electron) mobility \( \mu_{h(e)} \) are simple and accurate.

In the following, we will determine the minority-hole saturation-current density \( j_{ho} \), injected into the heavily doped n-type emitter-region of the p+-n junction solar cells.

5. Minority-Hole Saturation Current Density

Let us first propose in the non-uniformly and heavily doped (NUHD) emitter region of donor-Si devices our expression for the effective Gaussian donor-density profile or the donor (majority-electron) density, defined in the emitter-width region W, by:
\[ \rho(x) = N \times \exp \left\{ -\left( \frac{x}{W} \right)^2 \times \ln \left[ \frac{N}{N_0(W)} \right] \right\} \equiv N \times \left[ \frac{N}{N_0(W)} \right]^{-\left( \frac{x}{W} \right)^2} \] (24)

where \( N_0(W) \equiv 7.9 \times 10^{17} \times \exp \left\{ -\left( \frac{W}{0.1842 \mu m} \right)^{1.066} \right\} \) (cm\(^{-3}\)), 1 \( \mu m = 10^{-4} \) cm, decreases with increasing \( W \), in good agreement with the doping profile measurement on silicon devices, studied by Essa et al. [13]. Moreover, Equation (24) indicates that:

(i) at the surface emitter: \( x = 0 \), \( \rho(0) = N \), defining the surface donor density, and

(ii) at the emitter-base junction: \( x = W \), \( \rho(W) = N_0(W) \), which decreases with increasing \( W \), as noted above. Here, we also remark that \( N_0(VC) \equiv 7 \times 10^{17} \) cm\(^{-3}\) was proposed by Van Cong and Debiais (VCD) [22], and \( N_0(ZA) \equiv 2 \times 10^{18} \) cm\(^{-3}\), by Zouari and Arab (ZA) [17], for their Gaussian impurity density profile. Moreover, all the parameters given in Equation (24) were chosen such that the errors of our obtained \( j_{ho} \)-values are minimized, as seen in Table 4, and our numerical calculation indicates that, from Equation (24), we can determine the highest surface value, \( N_0 \), being equal here to 85 \( \mu m \).

Now, from Equations (8, 9) or Equation (19), taken for \( 0 \leq x \leq W \), and using Equation (24), the result: \( N_{\text{def}}(x = 0) \equiv N/\exp \left\{ \Delta E_g(N) \right\}_{k_BT} \) may be rewritten as:
\[ N_{\text{def}}(x) \equiv \rho(x)/\exp \left\{ \Delta E_g(p(x)) \right\}_{k_BT} \] (25)

which gives at \( x = W \): \( N_{\text{def}}(W) \equiv N_0(W)/\exp \left\{ \Delta E_g(N_0(W)) \right\}_{k_BT} \).

Then, under low-level injection, in the absence of external generation, and for the steady-state case, we can define the minority-hole density by:
\[ p_0(x) \equiv \frac{n^+}{N_{\text{def}}(x)} \] (26)

and a normalized excess minority-hole density [or a relative deviation between \( p(x) \) and \( p_0(x) \)] by [22, 25]:
\[ u(x) \equiv \frac{p(x) - p_0(x)}{p_0(x)} \] (27)

which must verify the two following boundary conditions proposed by Shockley as [2]:
\[ u(x = 0) \equiv -\frac{j_h(x=0)}{e S N_{\text{def}}(x=0)} \] (28)
\[ u(x = W) \equiv \exp \left( \frac{V}{n(V) \times V_T} \right) - 1, \text{for small } W - \text{values} \] (29)

Here, \( n(V) \) is an ideality factor, \( S (\text{cm}^2) \) is the hole surface recombination velocity at the emitter contact, \( V \) is the applied voltage, \( V_T \equiv (k_B T/e) \) is the thermal voltage, and the minority-hole current density \( j_h(x) \), being found to be similar to the Fick’s law for diffusion equation, is given by [8, 22]:
\[ j_h(x) = \frac{e n^+}{F(x)} \times \frac{du(x)}{dx} = \frac{-e n^+}{N_{\text{def}}(x) \times \tau_h(p(x))} \times \left[ \rho(x) - p_0(x) \right] \times \frac{1}{\tau_h(N)} \times \frac{1}{\tau_h(N)} \] (30)

Then, from these two Equations (30, 31), one obtains the following second-order differential equation as [22]:
\[ \frac{d^2 u(x)}{dx^2} - \frac{dF(x)}{dx} \times \frac{du(x)}{dx} - \frac{u(x)}{L_e^2} = 0 \] (32)

Using the two boundary conditions (28, 29), one thus gets the general solution of this Equation (32) as [22]:
\[ u(x) = \left( A(W) \times \sinh(P(x)) + B(W) \times \cosh(P(x)) \right) \times \left( \exp \left( \frac{V}{n(V) \times V_T} \right) - 1 \right) \] (33)

where \( A(W) \equiv \frac{1}{\sinh(P(W)) + I(W,S) \times \cosh(P(W))} \), \( I(W,S) \equiv \frac{B}{A} = \frac{D_h(N_0(W))}{S \times L_e(N_0(W))} \) and \( P(x) \equiv \int_0^x C \times F(x) \, dx \), since \( \frac{dF(x)}{dx} \equiv C \times F(x) \). Here, \( C = 10^{-17} \) (cm\(^3\)/s), as that chosen in Equation (20), and the hyperbolic sine-and-cosine functions are defined by: \( \sinh(x) \equiv 0.5 \times \left[ e^x - e^{-x} \right] \) and \( \cosh(x) \equiv 0.5 \times \left[ e^x + e^{-x} \right] \).

Further, from Eq. (33), as \( P(W) \ll 1 \) (or for small \( W \)) one has: \( A \approx \frac{1}{2} \) or \( B \approx 1 \), and one therefore obtains: \( u(W) = \left[ \exp \left( \frac{V}{n(V) \times V_T} \right) - 1 \right] \), which is just the boundary condition given in Equation (29). Now, using Equations (30, 33), one gets:
where $I_{h0}$ is the minority-hole saturation current density, being injected into the heavily doped n-type emitter region for $0 \leq x \leq W$ and given by:

$$I_{h0}(x, N, T, r_d, g_c, S) = -J_{h0}(x, N, T, r_d, g_c, S) \times \left( \frac{\exp \left( \frac{V}{n(V) + x} \right) - 1}{V} \right)$$

(34)

One also remarks that, from Equations (20, 33-35) and after some manipulations, one gets: $u(x = 0) \equiv \frac{I_{h0}(x = 0)}{eS \times h(x = 0)}$, being just the boundary condition given in Eq. (28). Now, using the $P(x)$-definition given in Equation (33), at $T=300$ K, one can define the inverse minority-hole diffusion length

$$\frac{1}{I_{h, \text{eff}}(x=W, N, T, r_d, g_c)} = \frac{W}{I_{h0}(x=W)} \int_{L_{h, \text{eff}}(x=W)} W \ dx \equiv \frac{W}{I_{h0}(x=W)} \int_{L_{h, \text{eff}}(x=W)} W \ C \times F(x) \ dx \equiv P(x=W, N, T, r_d, g_c) / W$$

(36)

where $I_{h0} = (CF)^{-1}$ is defined in Equation (20), in which $N$ is replaced by $h(x)$, being determined in Equation (24). Therefore, Equation (36) can be rewritten as:

$$P(x=W, N, r_d, g_c) \equiv \frac{W}{I_{h, \text{eff}}} = \frac{W}{L_{h, \text{eff}}} \times \frac{I_{h0}}{I_{h, \text{eff}}}$$

(37)

For a simplicity, Then, from Eq. (33, 35), since $B = A \times I(W, S)$ one obtains:

$$J_{h0}(x=0, N, r_d, g_c, S) = \text{en}_f C \times A = \frac{\text{en}_f C}{\sinh(P) + \times \cosh(P)}$$

(38)

$$J_{h0}(x=W, N, r_d, g_c, S) = \text{en}_f C \times \frac{A}{\sinh(P) + \times \cosh(P)}$$

(39)

Now, from those results (34, 38, 39), one gets:

$$I_{h0}(x=0, N, r_d, g_c, S) \equiv I_{h0}(x=W, N, r_d, g_c, S) \equiv I_{h0}(x=W, N, r_d, g_c, S) \equiv \frac{1}{\cos(P) + \times \cosh(P)}$$

(40)

Further, using Equations (27, 33, 34) and going back to the minority-hole continuity equation defined in Equation (31), one gets:

$$I_{h0}(x=W) \times \left[ J_{h0}(x=W) - J_{h0}(x=0) = \frac{1}{\tau_{h}(N)} \times Q_{h, \text{eff}}(x=W, N) \right]$$

(41)

where $\tau_{h}(N, r_d, g_c)$ is determined in Equation (20), and $Q_{h, \text{eff}}(C / cm^2)$ is the effective excess minority-hole density given in the emitter region, defined by [22]:

$$Q_{h, \text{eff}}(x=W, N) \equiv \int_{x}^{W} e \times [p(x) - p_{0}(x)] \times \frac{\tau_{h}(N)}{\tau_{h}(0)} dx$$

(42)

Finally, from Equations (40, 41), if defining the effective minority-hole transit time by: $\tau_{h, \text{eff}}(x=W, N, S) \equiv Q_{h, \text{eff}}(x=W, N, r_d, g_c, S)$, one then obtains the reduced effective minority-hole transit time, as:

$$\frac{\tau_{h, \text{eff}}(x=W, N, r_d, g_c, S)}{\tau_{h}} = 1 - \frac{1}{1 - \frac{I_{h0}(x=W, N, r_d, g_c, S)}{I_{h0}(x=W, N, r_d, g_c, S)}}$$

(43)

Now, from above Equations (38-43), some important results can be obtained and discussed below.

5.1. Very Large $S(= 10^{56} \, \text{cm}^{-2})$, For Example) or $S \rightarrow \infty$ and $P \ll 1$ or $W \ll L_{h, \text{eff}}$

Here, various results can be investigated as follows.

(i) From Equations (38-40), since $I(W) = \frac{D_{h}(N_{\text{f}, h}(W)))}{S \times L_{h, \text{eff}}(N_{\text{f}, h}(W))} \rightarrow 0$ as $S \rightarrow \infty$, $I_{h0}(x=0, N, r_d, g_c, S) \equiv I_{h0}(x=W, N, r_d, g_c, S) \equiv \frac{1}{\cos(P) + \times \cosh(P)}$ since $P \ll 1$ or $I_{h0}(x=W, N, r_d, g_c, S) \rightarrow \infty$. Therefore, from Equation (43), one obtains:

$$\frac{\tau_{h, \text{eff}}(x=W, N, r_d, g_c, S) \rightarrow \infty}{\tau_{h}} \approx 0$$

suggesting a completely transparent emitter region (CTER).

(ii) Further, from Equations (18-20, 39), since $I \rightarrow 0$ and $P \ll 1$, the result (39) is now reduced to:

$$I_{h0}(x=W, N, r_d, g_c, S) \rightarrow \infty \equiv \frac{\text{en}_f C}{\sinh(P) + \times \cosh(P)}$$

(44)

being found to be independent of $S$ and $C$, since $\frac{I_{h0}}{I_{h, \text{eff}}}$ is independent of $S$ and $C$ as observed in Equations (20, 36), and noting that the ABGN-expression is determined by Equation (9) or by Equation (15).

Now, in the P-Si system, for $T = 300$ K, $r_d \equiv r_p$ and $g_c = 6.5, 4.9113$, our two numerical $I_{h0}$ -results are calculated, using Equations (44, 9) and (44, 15), and given in Table 4, in which the CTER -condition, $P \ll 1$ (or $\frac{h, \text{eff}}{\tau_{h}(0)} \ll 1$) is fulfilled, and we also compare them with modeling and measuring $I_{h0}$ -results investigated by del Alamo et al. (ASS) [10, 12]. One notes that their modeling $I_{h0}$-result [10], based only on two independent parameters: $N_{\text{Def}, h}/D_{h}$ and $L_{h, \text{eff}}$, can be obtained, for $I_{h, \text{eff}} = W$, from our above result (44). This could explain a great difference between their modeling results [10, 12], being accurate within 36%, and ours, accurate within 1.78%, for $g_c = 6$, as those observed in the following Table 4.

Table 4. Our present results of $I_{h0}(x=W, N) \equiv \frac{I_{h0}(x=W, N)}{I_{h0}(x=W, N, r_d, g_c, S)}$, expressed as functions of $N$ for $g_c = 6.5, 4.9113$, and their relative deviations (RDs), calculated by: $RD(\%) = 1 - (\text{Present} \ I_{h0}(x=W, N) / \text{Present} \ I_{h0}(x=W, N, r_d, g_c, S))$, where the $I_{h0}(x=W, N, r_d, g_c, S)-data$ are given in References 10 and 12, the theoretical ASS/$I_{h0}(x=W, N, r_d, g_c, S)-results$, obtained by Alamo et al. (ASS) [10, 12], and also their relative deviations.

<table>
<thead>
<tr>
<th>$N \times 10^{19} , \text{cm}^{-2}$</th>
<th>2.1</th>
<th>3.3</th>
<th>4.3</th>
<th>4.6</th>
<th>12</th>
</tr>
</thead>
<tbody>
<tr>
<td>$W , (\mu \text{m})$</td>
<td>0.20</td>
<td>1.00</td>
<td>2.60</td>
<td>0.66</td>
<td>0.20</td>
</tr>
<tr>
<td>$I_{h0}(S \rightarrow \infty)$-data</td>
<td>$3.2 \times 10^{-12}$</td>
<td>$8.3 \times 10^{-13}$</td>
<td>$1.1 \times 10^{-12}$</td>
<td>$2.8 \times 10^{-12}$</td>
<td></td>
</tr>
<tr>
<td>$ASS/ I_{h0}(S \rightarrow \infty)$-data</td>
<td>$3.6 \times 10^{-12}$</td>
<td>$1.1 \times 10^{-12}$</td>
<td>$1.5 \times 10^{-12}$</td>
<td>$2.8 \times 10^{-12}$</td>
<td></td>
</tr>
<tr>
<td>RD(%)</td>
<td>-12.5</td>
<td>-32.5</td>
<td>0</td>
<td>-36</td>
<td>-4.0</td>
</tr>
<tr>
<td>$N_d , (\text{cm}^{-3})$</td>
<td>$2.65 \times 10^{17}$</td>
<td>$1.82 \times 10^{15}$</td>
<td>$2.22 \times 10^{17}$</td>
<td>$1.60 \times 10^{16}$</td>
<td>$2.65 \times 10^{17}$</td>
</tr>
</tbody>
</table>
Table 4 indicates that:
(i) the maximal relative deviations (RDs) in absolute values between our results (44, 9) and the $J_{0x}$-data [10, 12] are found to be: 1.78% for $g_e=6$, 4.56% for $g_e=5$, and 5.07% for $g_e=4.9113$, and
(ii) the maximal RDs in absolute values between our results (44, 15) and the $J_{0x}$-data [10, 12] are given by: 2.42% for $g_e=6$, 5.49% for $g_e=5$, and 5.75% for $g_e=4.9113$. It suggests that our numerical results (44, 9) for $g_e=6$ are the best ones, since they are accurate within 1.78%. Further, one notes that our $\Delta E_{ga}$-expression given in Equation (9) was obtained, taking into account all the physical effects such as: those of donor size, heavy doping and Fermi-Dirac statistics,

$$\tau_{\text{eff}}(x = W, N, r_d, g_e, S) \sim \tau_h \times \frac{D_h(N_d(W))}{S \times L_h(N_d(W))} \times \frac{P}{2} \times \left( \frac{D_h(N_d(W))}{S \times L_h(N_d(W))} \times \frac{P}{2} \right)^2$$

and in the lowly doped case (i.e., $L_{h,\text{eff}} \approx L_h$):

$$\tau_{\text{eff}}(x = W, N, r_d, S) \equiv \tau_e = \frac{W}{S} + \frac{W^2}{2D_h} \approx \frac{W^2}{2D_h}, \text{ as } S \to \infty$$

being just a familiar expression given for the minority-hole transit time $\tau_e$ obtained by

while in Equation (15) our $\Delta E_{ga}^{(\text{Mod.YC})}$-expression is only an empirical one. So, in the following, we will choose: $g_e=6$, $T=300$ K, and our ABGN-expression (9), for all the numerical calculations.

(iii) Furthermore, in particular, for large $S$ and small $P$, from Equation (40) one gets:

$$\frac{I_{0x}(x=0, N, r_d, S)}{I_{0x}(x=W, N, r_d, S)} \approx \frac{1}{\cosh(P) + \sinh(P)} \approx 1 - \frac{D_h(N_d(W))}{S \times L_h(N_d(W))} \times P - \frac{P^2}{2}$$

Then, from Equation (43), using Equations (20, 37) one obtains in the heavily doped case:

$$\tau_{\text{eff}}(x = W, N, r_d, g_e, S) \approx \tau_h \times \frac{D_h(N_d(W))}{S \times L_h(N_d(W))} \times \frac{P}{2} \times \left( \frac{D_h(N_d(W))}{S \times L_h(N_d(W))} \times \frac{P}{2} \right)^2$$

and in the lowly doped case (i.e., $L_{h,\text{eff}} \approx L_h$):

$$\tau_{\text{eff}}(x = W, N, r_d, S) \equiv \tau_e = \frac{W}{S} + \frac{W^2}{2D_h} \approx \frac{W^2}{2D_h}, \text{ as } S \to \infty$$

being just a familiar expression given for the minority-hole transit time $\tau_e$ obtained by

The underlined $|RD|$ values are the maximal ones.

5.2. Small $S = 10^{-50} \left( \text{cm}^3 \right)$ or $S \to 0$, and $P \gg 1$ or $W \gg L_{h,\text{eff}}$

Here, from Eq. (33) and for any $N$, one has: $I =$
\[
\frac{D_0(N_d(W))}{S_x L_0(N_d(W))} \rightarrow \infty, \text{ since } S \rightarrow 0.
\]
Therefore, from Equation (43), one obtains:
\[
\tau_{\text{eff}}(x = W, N, r_d, S) \equiv 1,
\]
suggesting a completely opaque emitter region (COER).

Now, our numerical results of \(J_{\text{EO}}(x = W, N, r_d, S) \equiv J_{\text{EO}}\) and \(\tau_{\text{eff}}(x = W, N, r_d, S) \equiv \tau_{\text{EO}}\), for simplicity, are respectively computed, using Equations (39) and (43), and then plotted into Figures 3 (a, a'), (b) and 4 (a', a'), (b) as functions of \(N\), and Figures 3 (c) and 4 (c), as functions of \(S\), noting that in those figures we also include various physical conditions such as: \(S, W, r_d\) and \(N\).

Figure 3. (a, a') Our \(J_{\text{EO}}\) results obtained as functions of \(N\), with a condition: \(N > N_{\text{EO}}(r_d)\), given in heavily doped donor-Si systems, as defined in Table 1, (b) ours obtained as a function of \(N\), and (c) ours obtained as a function of \(S\).
Some concluding remarks are obtained and discussed below.

(i) Figures 3(a1, a2) and 4(a1, a2) indicate that, since as $S \to \infty$ and $W = 1 \, \mu m$, $\tau_{th}$ decreases ($<4 \times 10^{-8}$) $\approx 0$, according to the CTER, and for a given $N$, due to the donor-size effect, both $J_{EO}$ and $\tau_{th}$ decrease (i) with increasing $r_d$. Then, for a given $r_d$, at large values of $N \geq 3 \times 10^{20} \, cm^{-3}$, due to the heavy doping effect, $J_{EO}$ (or $\tau_{th}$) increases (or decreases) with increasing $N$.

(ii) Figures 3(b) and 4(b) show that, for a given $N$, $J_{EO}$ (or $\tau_{th}$) decreases (or increases) with increasing $W$.

(iii) Figures 3(c) and 4(c), suggest that, for given $S$, $J_{EO}$ (or $\tau_{th}$) decreases (or increases) with increasing $W$.

(iv) In particular, in Figure 4(c), as $S \to 0$ and $W = 85 \, \mu m$, $\tau_{th}$ increases ($\to 1$), according to the COER.

Finally, it should be noted that in next Section 6 we must know the numerical results of dark saturation current density, defined by:

$$J_0(x = W, N, r_d, S, N_d, r_a) \equiv J_{EO}(x = W, N, r_d, S) + J_{BO}(N_d, r_a) \quad (47)$$

where $J_{BO}$ and $J_{EO}$ are determined respectively in Equations (21, 39). Then, those are tabulated in the following Table 5, in which all the physical conditions are also presented.

Table 5. Our numerical results of $J_0 = J_{EO} + J_{BO}$, calculated using Equation (47), where $J_{BO}$ and $J_{EO}$ are determined respectively in Equations (21, 39), and those are obtained in the three following cases.

<table>
<thead>
<tr>
<th>Case</th>
<th>Condition</th>
<th>$J_{EO}$ $= 6.0912 \times 10^{-13}$ $\left(\frac{A}{cm^2}\right)$</th>
<th>$J_{BO}$ $= 6.0912 \times 10^{-13}$ $\left(\frac{A}{cm^2}\right)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>First case</td>
<td>In the heavily doped (HD) P-Si emitter region ($N = 10^{20} , cm^{-3}$), and in the lightly doped (LD) B-Si base region ($N_a = 10^{16} , cm^{-3}$) in which $J_{EO} = 6.0912 \times 10^{-13}$ $\left(\frac{A}{cm^2}\right)$. For $S = 10^{10} , cm/s$ and $W = 0.206 , nm$, according to the completely transparent emitter region, one has: $J_{EO} = 2.4833 \times 10^{-10}$ $\left(\frac{A}{cm^2}\right) \gg J_{BO}$ and $I_a = 2.4839 \times 10^{-9}$ $\left(\frac{A}{cm^2}\right) \approx J_{EO}$ For $S = 10^{10} , cm/s$ and $W = 4.4 , nm$, according also to the completely transparent emitter region, one has: $J_{EO} = 1.1645 \times 10^{-10}$ $\left(\frac{A}{cm^2}\right) \gg J_{BO}$ and $I_a = 1.1706 \times 10^{-10}$ $\left(\frac{A}{cm^2}\right) \approx J_{EO}$ For $S = 10^4 , cm/s$ and $W = 0.36 , \mu m$, one has: $J_{EO} = 1.2237 \times 10^{-13}$ $\left(\frac{A}{cm^2}\right) \approx J_{BO}$ and $I_a = 7.3488 \times 10^{-13}$ $\left(\frac{A}{cm^2}\right) \approx J_{EO}$ For $S = 10^{-5} , cm/s$ and $W = 85 , \mu m$, according also to the completely opaque emitter region, one has: $J_{EO} = 4.7171 \times 10^{-19}$ $\left(\frac{A}{cm^2}\right) \ll J_{BO}$ and $I_a = 6.0912 \times 10^{-13}$ $\left(\frac{A}{cm^2}\right) = J_{BO}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Second case</td>
<td>In the completely opaque HD S-Si emitter region ($N = 5 \times 10^{20} , cm^{-3}$, $S = 10^{10} , cm/s$ and $W = 85 , \mu m$), and in the lightly doped a-Si base region, in which $N_a = 10^{16} , cm^{-3}$.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Third case</td>
<td>In the completely transparent HD d-Si emitter region ($N = 5 \times 10^{20} , cm^{-3}$, $S = 10^{10} , cm/s$ and $W = 0.000206 , \mu m$), and in the lightly doped Ti-Si base region, in which $N_a = 10^{16} , cm^{-3}$ and $J_{BO} = 5.3080 \times 10^{-17}$ $\left(\frac{A}{cm^2}\right)$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Some important remarks are given and discussed below.

(i) In the first case, with decreasing S and increasing W, $I_{o}$ thus decreases from the CTER to the COER, and one gets in this COER: $I_{o} = I_{BO}$.

(ii) In the second case or in the COER-conditions, $I_{BO}$ decreases with increasing $r_{a}$, being due to the acceptor-size effect, and for given $r_{a}$ one has: $I_{o} = I_{BO}$ since $I_{Eo} = 0$.

(iii) In the third case or in the CTER-conditions, $I_{Eo}$ decreases with increasing $r_{d}$, being due to the donor-size effect, and for (r$_{a}$, r$_{T1}$), one gets: $I_{o} = J_{BO} = 5.3080 \times 10^{-17} \frac{A}{cm^2}$, which can be compared with the similar result, obtained the second case or in the COER-conditions, as: $I_{o} = J_{BO} = 5.3080 \times 10^{-17} \frac{A}{cm^2}$, calculated for (r$_{o}$, r$_{T1}$).

It should be noted that these values of $I_{o}$ will strongly affect the variations of various photovoltaic conversion parameters of n$^{+}$-p junction silicon solar cells, such as: the ideality factor $n$, short circuit current density $I_{SC}$, fill factor FF, and photovoltaic conversion efficiency $\eta$, being expressed as functions of the open circuit voltage, $V_{oc}$ [4], as investigated in the following. Our empirical treatment method used is that of two points. The first point is characterized by [27]:

$$V_{oct} = 624 \text{ mV}, I_{sc1} = 36.3 \frac{mA}{cm^2}, FF_{1} = 80.1 \% \quad (48)$$

Here, $n$ is the ideality factor, being determined by our empirical treatment method of two points, as:

$$n(W, N, r_{d}, S, N_{a}, r_{a}, V_{oc}) = n_{1}(W, N, r_{d}, S, N_{a}, r_{a}, V_{oc1}, I_{sc1}) + n_{2}(W, N, r_{d}, S, N_{a}, r_{a}, V_{oc2}, I_{sc2}) \times \left(\frac{V_{oc}}{V_{oc1}} - 1\right)^{y_{n}},$$

$$y_{n} = 1.1248 \quad (52)$$

which is valid for any $W, N, r_{d}, S, N_{a}, r_{a}, V_{oc} \geq V_{oc1}$, and increases with increasing $V_{oc}$ for given $W, N, r_{d}, S, N_{a}$ and $r_{a}$.

Further, the values of $V_{oc1}$, $I_{sc1}$, $V_{oc2}$ and $I_{sc2}$ are given in Equations (48, 49), and the numerical results of $n_{1(2)}$ can be determined from Equation (51) by:

$$n_{1(2)}(W, N, r_{d}, S, N_{a}, r_{a}, V_{oc1(2)}, I_{sc1(2)}) \equiv \frac{V_{oc1(2)}}{V_{T}} \times \frac{1}{ln \left(\frac{V_{oc1(2)}}{V_{T}}\right)} \quad (53)$$

implying that both $n_{1(2)}$ (or n) and $I_{o}$ have the same variations for given $(W, N, r_{d}, S, N_{a}, r_{a})$-variations, being found to be an important remark.

Furthermore, in Equation (52), for the CTER-conditions such as:

$$W = 4.4 \text{ nm} = 0.0044 \mu m, N = 10^{20} \text{ cm}^{-3}, r_{d} = r_{p}, S = 10^{50} \text{ cm}^{2} \text{ s}, N_{a} = 10^{16} \text{ cm}^{-3}, r_{a} = r_{B}$$

the exponent $y_{n} = 1.1248$ was chosen such that:

$$n(W, N, r_{d}, S, N_{a}, r_{a}, V_{oct1(2)}) \equiv n_{1(2)}(W, N, r_{d}, S, N_{a}, r_{a}, V_{oc1(2)}, I_{sc1(2)}) = 1.2344 (1.4534)$$
For example, from the above remark given in Eq. (53) and from the first case reported in Table V, we can conclude that, with decreasing S and increasing W, both n and J_{sc} decrease from the CTER to the COER. Therefore, from Equation (51), J_{sc} thus increases from the CTER to the COER, since J_{sc} is expressed in terms of \( e^{\frac{V_{oc}}{n \cdot V_r}} \).

Then, the values of the fill factor FF for \( V_{oc} = V_{oc1(2)} \) can be found to be given by:

\[
FF_{1(2)}(W, N, r_d, S, N_p, r_a, V_{oc1(2)}) = \frac{v(W, N, r_d, S, N_p, r_a, V_{oc1(2)})}{v(W, N, r_d, S, N_p, r_a, V_{oc1(2)}) + 0.72} \times y_{FF}
\]

(55)

where \( z_{FF1(2)} = 1.1 \) \((0.472)\) was chosen such that, under the above conditions (54), the values of \( FF_{1(2)} \), calculated using Equation (55), are identical to the data given in Equations (48, 49); 80.1% \((82.7\%)\), respectively [27, 23].

Moreover, in the case where both series resistance and shunt resistance have a negligible effect upon cell performance, \( z_{FF1(2)} \), Green \([4]\), was chosen such as 1, as proposed by Green [4].

Now, by applying a same above treatment method of two points, one has:

\[
y_{FF} = 2.0559
\]

(56)

which is valid for any \( W, N, r_d, S, N_p, r_a, V_{oc} \geq V_{oc1} \), and increases with increasing \( V_{oc} \) for, given \( W, N, r_d, S, N_p, \) and \( r_a \). Here, the value of \( y_{FF} = 2.0559 \) was chosen such that, under the conditions (54), \( FF(W, N, r_d, S, N_p, r_a, V_{oc1}) \equiv FF_{1(2)}(W, N, r_d, S, N_p, r_a, V_{oc1(2)}) = 80.1\% \((82.7\%)\) \), respectively [27, 23].

Then, the photovoltaic conversion efficiency \( \eta \) can be defined by:

\[
\eta(W, N, r_d, S, N_p, r_a, V_{oc}) = \frac{J_{sc} \times V_{oc} \times FF}{P_{in}}
\]

(57)

where \( J_{sc} \) and \( FF \) are determined respectively in Equations (51, 56), being assumed to be obtained at 1 sun illumination or at AM1.5G spectrum \((P_{in} = 0.100 \frac{W}{cm^2}) [27, 28]\).

\[
W = 0.206 \text{nm}, N = 10^{20} \text{cm}^{-3}, r_d \equiv r_P, S = 10^{50} \text{cm}^{-3}, N_a = 10^{16} \text{cm}^{-3}, r_a \equiv r_B
\]

(58)

according to the CTER, we get the precisions of the order of 8.1% for \( J_{sc} \), 7.1% for \( FF \), and 5% for \( \eta \) calculated using the corresponding data [23, 24, 27-29], which is strongly affected by \( J_0 = J_{po} + J_{bo} \), as noted above, suggesting thus an accuracy of \( J_{bo} \leq 8.1\% \), since \( J_{bo} \) was accurate within 1.78%, as given in Table 4.

<table>
<thead>
<tr>
<th>Data (D) from References</th>
<th>( V_{oc} ) (mV)</th>
<th>n</th>
<th>( J_{sc(PP)}(J_{sc(D)}); \text{RD}) )</th>
<th>( FF_{PP}(%); \text{RD}) )</th>
<th>( \eta_{PP}(%); \text{RD}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>[28]</td>
<td>750</td>
<td>1.7474</td>
<td>40.24 (39.5); 1.9</td>
<td>80.58 (83.2); 3.1</td>
<td>24.32 (24.7); 1.5</td>
</tr>
<tr>
<td>[23, 28]</td>
<td>740</td>
<td>1.7222</td>
<td>40.01 (41.8); 1.9</td>
<td>80.11 (82.7); 3.1</td>
<td>24.31 (25.6); 5.0</td>
</tr>
<tr>
<td>[28]</td>
<td>738</td>
<td>1.7172</td>
<td>41.16 (40.8); 0.9</td>
<td>80.02 (83.5); 4.2</td>
<td>24.31 (25.1); 3.2</td>
</tr>
<tr>
<td>[28]</td>
<td>737</td>
<td>1.7146</td>
<td>41.23 (41.3); 0.2</td>
<td>80.00 (82.7); 3.3</td>
<td>24.30 (25.2); 3.6</td>
</tr>
<tr>
<td>[28]</td>
<td>718</td>
<td>1.6676</td>
<td>42.43 (42.1); 0.8</td>
<td>79.22 (83.2); 4.8</td>
<td>24.13 (25.1); 3.8</td>
</tr>
<tr>
<td>[24]</td>
<td>710</td>
<td>1.6481</td>
<td>42.82 (43.2); 1.2</td>
<td>78.95 (82.6); 4.4</td>
<td>24.00 (24.8); 3.2</td>
</tr>
<tr>
<td>[28, 29]</td>
<td>706</td>
<td>1.6384</td>
<td>42.98 (42.7); 0.6</td>
<td>78.82 (82.8); 4.8</td>
<td>23.91 (25.0); 4.3</td>
</tr>
<tr>
<td>[24]</td>
<td>705</td>
<td>1.6360</td>
<td>43.02 (42.2); 1.9</td>
<td>77.87 (83.1); 6.3</td>
<td>23.89 (24.7); 3.3</td>
</tr>
<tr>
<td>[24]</td>
<td>703</td>
<td>1.6312</td>
<td>43.08 (42.0); 2.6</td>
<td>78.73 (82.7); 4.8</td>
<td>23.84 (24.4); 2.3</td>
</tr>
<tr>
<td>[28]</td>
<td>695</td>
<td>1.6122</td>
<td>43.30 (40.2); 7.7</td>
<td>78.50 (80.5); 2.5</td>
<td>23.62 (22.5); 4.9</td>
</tr>
<tr>
<td>[28]</td>
<td>680</td>
<td>1.5772</td>
<td>43.37 (40.5); 7.1</td>
<td>78.14 (80.3); 2.7</td>
<td>23.05 (22.1); 4.3</td>
</tr>
<tr>
<td>[29]</td>
<td>671.7</td>
<td>1.5584</td>
<td>43.20 (40.5); 6.5</td>
<td>77.98 (80.9); 3.6</td>
<td>22.63 (22.0); 2.8</td>
</tr>
<tr>
<td>[28]</td>
<td>667</td>
<td>1.5479</td>
<td>43.01 (39.8); 8.1</td>
<td>77.91 (80.0); 2.6</td>
<td>22.35 (21.3); 4.9</td>
</tr>
<tr>
<td>[27]</td>
<td>665</td>
<td>1.5434</td>
<td>43.91 (42.2); 1.7</td>
<td>76.87 (78.7); 1.0</td>
<td>22.22 (22.1); 0.5</td>
</tr>
</tbody>
</table>

\(^{\text{Table 6. With the physical conditions given in Equation (58), our present results (PR) of \( n, J_{sc}, FF \), and \( \eta \), calculated using Equations (52, 51, 56, 57), being compared with corresponding data [23, 24, 27-29], and their relative deviations (RD), computed using the formula: \( \text{RD} = \left| 1 - \frac{\text{PR}}{\text{Data}} \right| \).}\)}
In Figures 5 (a), (b), (c) and (d), the physical conditions used are:

\[ N = 10^{20} \text{ cm}^{-3}, r_d = r_p, N_a = 10^{16} \text{ cm}^{-3}, r_a = r_B, \text{and different } (S, W) \text{ values} \quad (59) \]

which are given also in these figures, and in Table 5 for the first case. Here, for a given \( V_{oc} \), and with decreasing \( S \) and increasing \( W \), we observe that:

(i) in the Figure 5 (a), the function \( n \) determined in Equation (52) (or the function \( I_o \) given in Table 5) decreases from the CTER to the COER

(ii) in Figures 5 (b), 5 (c) and 5(d), the functions \( J_{sc}, FF \) and \( \eta \) therefore increase from the CTER to the COER, and

(iii) in Figure 5 (d), for the physical functions: \( W=85 \mu m \) and \( S = 10^{-50} \text{ cm/s} \), the function \( \eta \) reaches a maximum equal to 27.77\% at \( V_{oc} = 715 \text{ mV} \); here \( 1 \mu m = 10^{-6} \text{ m} \).

In Figures 6 (a), (b), (c) and (d), the physical conditions used are:

\[ W = 85 \mu m, N = 5 \times 10^{20} \text{ cm}^{-3}, r_d = r_p, S = 10^{-50} \text{ cm/s}, \]

\[ N_a = 10^{16} \text{ cm}^{-3}, r_a \text{, and } E_{gl}(r_a) \text{ at 300 K} \quad (60) \]

according to the COER, and they are also given in these
figures and in Table 5 for the second limiting case, in which $I_0 = I_{B_0}$, since $I_{E_0} = 0$. Thus, this simplifies the numerical calculation of functions $n$, $I_{sc}$, FF and $\eta$, using Equations (52, 51, 56, 57), where $I_0$ is replaced by $I_{B_0}$, determined by Eq. (21). Further, in Equation (60), the values of $E_{gl}(r_d)$ are given in Table 2. Then, for a given $V_{oc}$ and with increasing $r_d$-values, it should be concluded that, due to the acceptor-size effect,

(i) in the Figure 6 (a), the function $n$ determined in Equation (52) (or the function $J_0$ given in Table 5) decreases (↓), and

(ii) in Figures 6 (b), (c), (d), the functions $I_{sc}$, FF and $\eta$ therefore increase (↑), and in particular, in Figure 6 (d), for the completely opaque (S-Si) emitter-region conditions, where $I_{E_0} = 0$ or $I_0 = I_{B_0}$, the maximal $\eta$-values are equal to: 27.77 %, …, 31.55 %, at $V_{oc} = 715$ mV, …, 703 mV, according to the $E_{gl}$-values equal to: 1.12 eV, …, 1.34 eV, which are obtained in various lightly doped (B, …, Tl)-Si base regions, respectively, being due to the acceptor-size effect.

Finally, in Figures 7 (a), (b), (c) and (d), the physical conditions used are:

$W = 0.000206 \, \mu m, N = 5 \times 10^{20} \, cm^{-3}, r_{B_0} \cdot S = 10^{50} \, cm \, s^{-1}, $ 
$N_a = 10^{16} \, cm^{-3}, r_{T_1}, $ and $E_{gl}(r_d)$ at 300 K (61)

decreases (↓), and

(i) in the Figure 7 (a), the function $n$ determined in Equation (52) (or the function $I_0$ given in Table 5) decreases (↓), and

(ii) in Figures 7 (b), (c), (d), the functions $I_{sc}$, FF and $\eta$ therefore increase (↑), and in particular, in Figure 7 (d), in the conditions of completely transparent and heavily doped (donor-Si) emitter-and- lightly doped (Tl-Si) base regions, the maximal $\eta$-values are equal to:
24.28 %, ..., 31.51 %, at $V_{oc} = 748$ mV, ..., 703 mV, according to the $E_g$-values equal to: 1.11 eV, ..., 1.70 eV, obtained in various (Sb, ..., S)-Si emitter regions, respectively, being due to the donor-size effect, which can be compared with those given in Figure 6 (d).

![Graph](image)

Figure 7. For $N = 5 \times 10^{20}$ cm$^{-3}$ and $N_d = 10^{16}$ cm$^{-3}$, (a) our $n$-results, (b) $J_{oc}(V_{oc})$-results, (c) FF($\%$)-results, and (d) $\eta$($\%$)-results, plotted as functions of $V_{oc}$ and obtained in the CTER-conditions.

7. Concluding Remarks

We have developed the effects of heavy doping and impurity size on various parameters at 300 K, characteristic of energy-band structure, as given in Sections 2 and 3, and of the performance of crystalline silicon solar cells, being strongly affected by the dark saturation current density: $J_0 \equiv J_{oc} + J_{bo}$, as given in Sections 4, 5 and 6. Then, some concluding remarks are obtained and discussed as follows.

1. Using the OPG ($E_g$)-data given by Wagner and del Alamo [44], our $E_g$-results, due to the heavy doping effect, and calculated using Equation (16), are found to be accurate within 1.86%, as observed in Table 3.

2. In the CTER-conditions, as those given in Table 4, and using the $J_{sc}$-data, given by del Alamo et al. [10, 12], by using Equation (44), our $J_{sc}$-results, obtained in the heavily doped and completely transparent (P-Si) emitter region, are found to be accurate within 1.78%, while the modeled $J_{sc}$-results, obtained by those authors, are accurate within 36% [10, 12].

3. For given physical conditions and using an empirical treatment method of two points, as developed and discussed in Section 6, both our two results ($n$ and $J_0$) have the same variations, which strongly affect other ($V_{oc}$, $J_{sc}$, FF, $\eta$)-results, as discussed in Eq. (53). Thus, $J_0$, determined in Equation (47), is a central result of our present paper.

4. In the CTER-conditions, as those given in Equation (58), and using various ($J_{sc}$, FF, $\eta$)-data [23, 24, 27-29], we get the precisions of the order of 8.1% for $J_{sc}$, 7.1% for FF and 5% for $\eta$, suggesting thus a probable accuracy of $J_{bo}$ ($\leq 8.1\%$), since our $J_{bo}$-results are accurate within 1.78%.

5. In the physical conditions of completely opaque and heavily doped (S-Si) emitter-and-lightly doped (acceptor-Si) base regions, as given in Eq. (60), and in the physical conditions of completely transparent and heavily doped (donor-Si) emitter-and-lightly doped (Tl-
Si) base regions, as given in Eq. (61), our obtained
maximal η-values, due to the impurity-size effect, are
found to be equal respectively to: 27.77%, ..., 31.55%,
as seen in Figure 6 (d), and 24.28%, ..., 31.51%, as
observed in Figure 7 (d), suggesting that our obtained
highest η-values are found to be almost equal, as:
31.51% ≈ 31.55% , since the two corresponding
limiting \( f_0 \)-values are almost the same, as given in
Table 5, for second and third cases.

In summary, being due to the impurity-size effects, our
limiting value of \( \eta = 31.55% \), as that given in Figure 6 (d), is
thus obtained in the following limiting physical conditions as:
\[
W = 85 \, \mu m, N = 5 \times 10^{20} \, \text{cm}^{-3}, E_{\text{g}}(r_d = r_s) = 1.7035 \, eV, S = 10^{-50} \, \text{cm}^{-5} \text{eV},
\]
\[
N_s = 10^{16} \, \text{cm}^{-3}, \text{and } E_{\text{g}}(r_s) = 1.3415, \text{at } 300 \, K,
\]
and \( \eta = 27.77% \), as that given in Figure 5 (d), is obtained in
the following limiting physical conditions as:
\[
W = 85 \, \mu m, N = 10^{20} \, \text{cm}^{-3}, E_{\text{g}}(r_d = r_p) = 1.1245 \, eV, S = 10^{-50} \, \text{cm}^{-5} \text{eV},
\]
\[
N_s = 10^{16} \, \text{cm}^{-3}, \text{and } E_{\text{g}}(r_s) = 1.1245, \text{at } 300 \, K.
\]

Those limiting \( \eta_{1,2} \)-results can be compared with that
obtained by Richter et al. (R) [26], \( \eta = 29.43\% \), for a thick
100 \( \mu m \) solar cell made of un-doped silicon, as:
\( \eta_2 < \eta_R < \eta_1 \).

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greatly improved the presentation of our paper.

Appendix

Appendix A: Fermi Energy

The Fermi energy \( E_F \), obtained for any \( T \) and donor
density \( N \), being investigated in our previous paper, with
a precision of the order of \( 2.11 \times 10^{-4} \) [39], is now
summarized in the following. First of all, we define the
reduced electron density by:
\[
\bar{u}(N, T, r_d, g_c) \equiv \frac{N}{N_c(T, r_d, g_c)} = F_{1/2}(\theta) \tag{A1}
\]
where \( N_c \) is defined in Eq. (6), \( \theta(u) \equiv \frac{E_{\text{F}}(u)}{k_B T} \) is the reduced
Fermi energy, and \( F_{1/2}(\theta) \) is the Fermi-Dirac integral,
declared by [40]:
\[
\frac{F_{1/2}(\theta)}{2} \equiv \frac{2}{\sqrt{\pi}} \int_0^{+\infty} \frac{1}{1 + e^{\theta x}} x \equiv \frac{E}{k_B T} \tag{A2}
\]
which was calculated for any values of \( \theta \), with a precision
of the order of \( 10^{-7} \), by Van Cong and Doan Khanh [40], using
a theorem existence of Hermite interpolating polynomials.

Then, by a reversion method of \( u \equiv F_{1/2}(\theta) \) so useful to
obtain \( \theta(u) \), concerned with doped semiconductors at
arbitrary \( N \) and \( T \), our expression for reduced Fermi energy
was found to be given by [39]:
\[
\theta(u) \equiv \frac{E_{\text{F}}(u)}{k_B T} = \frac{G(u) + \mu^\theta P(u)}{1 + \mu^\theta a^\theta}, \text{with } \lambda = 0.0005372 \text{ and } B = 4.82842262 \tag{A3}
\]
where, in the degenerate case or when \( \theta(u) < 1 \) → ∞ ,
Equation (A3) is reduced to:
\[
F(u) = au^2 \left( 1 + bu^4 + cu^6 + d \right); \text{ with } \lambda = \left[ 3\sqrt{\pi}/4 \right]^{2/3}, \text{ and } b = \frac{1}{8}(\pi^2)^{2/3}, \text{ and } c = \frac{2\pi}{9\sqrt{3}} \tag{A4}
\]
and we express the effective Wigner-Seitz radius \( r_s \)
characteristic of the interactions by:
\[
r_s(N, T, r_d, g_c) \equiv \frac{3g_e^2}{4\pi N} \times \frac{1}{a_B(T, r_d)} \tag{A5}
\]
Here, \( a_B(T, r_d) = 5.2917715 \times 10^{-9} \times \frac{e(r_d)}{m_e(T, r_d)} \text{ (cm)} \) is
the Bohr radius. Therefore, one has:
\[
r_s(N, T, r_d, g_c) = 1.1723 \times 10^8 \times \left( \frac{E_{\text{F}}}{N} \right)^{1/3} \times \frac{m_e(T, r_d)}{e(r_d)} \tag{A6}
\]
and the ratio \( R/r_s \) is thus proportional to:
\[
\frac{e(r_d)}{m_e(T, r_d)} \times N_r^{1/3}, \text{ where } N_r \equiv \frac{6 \times 10^{17}}{G_{r}(9.999 \times 10^{17} \, \text{cm}^{-3})} \text{. Now, an empirical expression for BGN is proposed by:}
\]
\[
\Delta E_g(N, T, r_d, g_c) \equiv -R \times \mu_e(r_s) - R \times \mu_c(r_s) - R \times \mu_{e-d}^b(r_s) - R \times \mu_{c-d}^b(r_s) + \Delta E_g(LT) \tag{A7}
\]
where, \( R \) and \( r_s \) are defined above, and five first
contributions of the spin-polarized chemical potential energy
\( \mu \) determined in our previous paper [42], and sixth \( \mu^\theta \)-
one by Lanyon and Tuft [6]. One notes here that the second
\( -R \times \mu_c(r_s) \)-term of Equation (A6) represents the shift in
majority conduction-band edge, due to the correlation (Cor)
energy of an effective electron gas, \( E_c(r_s) \), as [42]:
\[
E_c(N, T, r_d, g_c) = \frac{0.087553 + 0.087553}{1 + 0.03847728 \times 10^{3} \times 10^{37} J} \times \ln(\theta_r - 0.095288) \tag{A8}
\]
and that from the a Seitz’s theorem [42], one has:
\[ \mu_c(N, T, r_d, g_c) \equiv -\frac{r_d}{3} \frac{\partial E_c(r_d)}{\partial g_c} - \frac{r_d}{3} \frac{\partial E_c}{\partial g_c} + \frac{2503}{3} \left[ E_c(r_d) \right] \equiv \mu_c(A_c)(r_d), \tag{A8} \]

being obtained with an accuracy of 1.87% for \( g_c = 6 \) in various donor-Si systems. Then, an approximate expression for the BGN is found to be given by:

\[
\Delta E_g(N, T, r_d, g_c) \approx a_1 \frac{\mu(T)}{m_c(T)} + a_2 \frac{\mu(T)}{m_c(T)} + a_3 \left( \frac{\mu_c(T, r_d)}{m_c(T, r_d)} \right)^{1/2} \times \\
N_r^{1/2} \left[ \frac{m_c(T, r_d)}{m_c(T, r_d)} \right] + a_4 \frac{\mu_c(T, r_d)}{m_c(T, r_d)} \times \left( \frac{\mu(T)}{m(T)} \right)^{1/2} \times \\
N_r^{1/2} \left[ \frac{m_c(T, r_d)}{m_c(T, r_d)} \right] + \frac{\mu_c(T, r_d)}{m_c(T, r_d)} \times \left( \frac{\mu(T)}{m(T)} \right)^{1/2} \times \\
N_r^{1/2} \left[ \frac{m_c(T, r_d)}{m_c(T, r_d)} \right] + a_5 \left( \frac{\mu_c(T, r_d)}{m_c(T, r_d)} \right)^{1/2} \times \left( \frac{\mu(T)}{m(T)} \right)^{1/2} \times N_r^{1/2} \tag{A9} \]

noting that, in the P-Si system for 300 K, these constants:

\[ a_1 = 3.8 \times 10^{-3} \, (eV), \quad a_2 = 6.5 \times 10^{-4} \, (eV), \quad a_3 = 2.8 \times 10^{-3} \, (eV), \quad a_4 = 5.597 \times 10^{-3} \, (eV), \quad \text{and} \quad a_5 = 8.1 \times 10^{-4} \, (eV), \]

were chosen such that for \( g_c = 6 \) the numerical results of minority-carrier saturation current \( J_{so} \) are found to be accurate within 1.78%, as seen in Table 4.

References


