SCIREA Journal of Physics

http://www.scirea.org/journal/Physics

July 15, 2019

Volume 4, Issue 4, August 2019

Effects of Heavy Doping and Impurity Size on Minority-Carrier Transport Parameters in Heavily (Lightly) Doped n(p)-Type Crystalline Silicon at 300 K, Applied to Determine the Performance of $n^{+}-p$ Junction Solar Cells

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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 η, 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 η, suggesting thus an accuracy of J_{Bo} $(\leq 8.1\%)$. 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 η-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 η-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 η-values are found to be almost equal, as: $31.51\% \simeq 31.55\%$, coming from the fact that the two obtained limiting J_o-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 η, 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 n(p)-type thin emitter region such as [1-45]: the band gap narrowing (BGN), ΔE_g, Fermi energy E_F, apparent band gap narrowing (ABGN), ΔE_{ga}, 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 (dilatation)], 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 ΔE_g, Fermi energy E_F, apparent band gap narrowing ΔE_{ga}, and effective intrinsic carrier concentration n_{ie}. In Section 3, an accurate expression for the optical band gap (OBG), E_{g1}, is investigated in next Equation (16), being accurate within 1.86%, as showed in Table 3. Some useful minority-carrier transport parameters such as: μ_h and L_h, being given in the heavily doped n-type emitter region, and μ_e, τ_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: $J_o = J_{Eo} + J_{Bo}$, 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, suggesting that:

(1) a precision of the order of 5% is obtained in the completely transparent emitter region case for the photovoltaic conversion efficiency η, as given in Table 6,

(2) in the conditions of completely opaque and heavily doped (S-Si) emitter-and-(acceptor-Si) lightly doped base regions, the maximal η-values 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, as those given in next Figure 8 (d), and

(3) in the conditions of completely transparent and heavily doped (donor-Si) emitter-and-lightly doped (Tl-Si) base regions, the maximal η-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, as those given in next Figure 9 (d).

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_o, assuming that in the P(B)-Si system $r_{P(B)} = r_o = 0.117$ nm, with $1\,nm = 10^{-9}m$, a local mechanical strain (or deformation potential energy) is induced, according to a compression (dilation) for $r_{d(a)} > r_o$ ($r_{d(a)} < r_o$), 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 (dilatation) 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, $E_{go}(r_{P(B)}) = 1.17$ eV, and effective d(a)-ionization energy in absolute values $E_{do(ao)}(r_{P(B)}) = 33.58$ meV, are obtained in an effective Bohr model, as [42]:

$$\begin{aligned} E_{go}(r_{d(a)}) - E_{go}(r_{P(B)}) &= E_{do(ao)}(r_{d(a)}) - E_{do(ao)}(r_{P(B)}) \\ &= E_{do(ao)}(r_{P(B)}) \times \left[\left(\frac{\varepsilon(r_{P(B)})}{\varepsilon(r_{d(a)})}\right)^2 - 1\right] \end{aligned} \quad (1)$$

Therefore, with increasing $r_{d(a)}$, the effective dielectric constant $\varepsilon(r_{d(a)})$ decreases, implying that $E_{go}(r_{d(a)})$ 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 $N_{cn(cp)}(r_{d(a)})$ are also reported. This critical density marks the metal-to-insulator transition from the localized side (all the impurities are electrical neutral), $N(N_a) \leq N_{cn(cp)}(r_{d(a)})$, to the extended side, $N(N_a) \geq N_{cn(cp)}(r_{d(a)})$, 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: $\mathrm{N(N_a)} > N_{\mathrm{cn(cp)}}(\mathrm{r_{d(a)}})$ and $\mathrm{N(N_a)} < N_{\mathrm{cn(cp)}}(\mathrm{r_{d(a)}})$, can thus be used to define the n(p)-type heavily and lightly doped Si, respectively.

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

Donor	***Sb***	***P***	***As***	***Bi***	***Ti***	***Te***	***Se***	***S***
				T=0 K				
$\mathrm{r_d}$ (nm)	0.1131	0.1170	0.1277	0.1292	0.1424	0.1546	0.1621	0.1628
$\varepsilon(\mathrm{r_d})$	12.02	11.40	8.47	7.95	4.71	3.26	2.71	2.67
$\mathrm{E_{go}(r_d)(eV)}$	1.167	1.170	1.197	1.205	1.333	1.547	1.729	1.749
$\mathrm{N_{cn}(r_d)(10^{18}\ cm^{-3})}$	3	3.52	8.58	10.37	50	150.74	261.24	274.57

At T=300 K, conditions: $\mathrm{N} > N_{\mathrm{cn}}(\mathrm{r_d})$ and $\mathrm{N} < N_{\mathrm{cn}}(\mathrm{r_d})$, can thus be used to define the n-type heavily (lightly) doped Si, respectively.

Acceptor	***B***	***Al***	***Ga***	***In***	***Tl***
			T=0 K		
$\mathrm{r_a}$ (nm)	0.1170	0.1254	0.1263	0.1352	0.1410
$\varepsilon(\mathrm{r_a})$	11.40	8.88	8.49	5.57	4.42
$\mathrm{E_{go}(r_d)}$ (eV)	1.170	1.195	1.201	1.292	1.387
$\mathrm{N_{cp}(r_a)(10^{18}\ cm^{-3})}$	4.06	8.58	9.83	34.73	69.87

At T=300 K, conditions: $\mathrm{N_a} > N_{\mathrm{cp}}(\mathrm{r_a})$ and $\mathrm{N_a} < N_{\mathrm{cp}}(\mathrm{r_a})$, can thus be used to define the p-type heavily (lightly) doped Si, respectively.

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, $\mathrm{E_{gi}(T, r_{d(a)})}$, by

$$E_{gi}\left(T,r_{d(a)}\right) \simeq E_{go}(r_{d(a)}) - 0.071\ (\mathrm{eV}) \times \left\{ \left[1 + \left(\frac{2T}{440.6913\ \mathrm{K}}\right)^{2.201} \right]^{\frac{1}{2.201}} - 1 \right\} \quad (2)$$

where the values of $E_{go}(r_{d(a)})$ due to the d(a)-size effect are given in Table 1 and those of $E_{gi}\left(T = 300\ \mathrm{K}, r_{d(a)}\right)$ tabulated in Table 2. Further, as noted in this Reference 43, in the (P, S)-Si systems, for $0\ \mathrm{K} \leq T \leq 3500\ \mathrm{K}$, the absolute maximal relative errors of this E_{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]:

$$m_c(T,r_d) = \left[0.9163 \times \left(0.1905 \times \frac{E_{go}(r_d)}{E_{gi}(T,r_d)} \right)^2 \right]^{1/3} \times m_o = m_{eo} \times \left(\frac{E_{go}(r_d)}{E_{gi}(T,r_d)} \right)^{2/3} \quad (3)$$

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

$$m_v(T) = g_v^{-2/3} \times \left(\frac{0.443587 + 0.3609528 \times 10^{-2}T + 0.1173515 \times 10^{-3}T^2 + 0.1263218 \times 10^{-5}T^3 \cdot}{1 + 0.4683382 \times 10^{-2}T + 0.2286895 \times 10^{-3}T^2 + 0.7469271 \times 10^{-6}T^3 + 0.} \right. \quad (4)$$

which gives $m_v(T = 0\ \mathrm{K}) = m_{vo} = 0.3664 \times m_o$. Here, $g_v = 2$ is the effective average number of equivalent valence-band edges.

Now, the intrinsic carrier concentration n_i is defined by

$$n_i^2(T,r_{d(a)},g_c) \equiv N_c(T,r_d,g_c) \times N_v(T,g_v) \times \exp\left(\frac{-E_{gi}\left(T,r_{d(a)}\right)}{k_B T} \right) \quad (5)$$

where, $N_{c(v)}$ is the conduction (valence)-band density of states, given by [31, 32]:

$$N_c(T,r_d,g_c) = 2g_c \times \left(\frac{m_c(T,r_d) \times k_B T}{2\pi\hbar^2} \right)^{\frac{3}{2}} (\mathrm{cm}^{-3}) \quad (6)$$

$$N_v(T,g_v) = 2g_v \times \left(\frac{m_v(T) \times k_B T}{2\pi\hbar^2} \right)^{\frac{3}{2}} (\mathrm{cm}^{-3}) \quad (7)$$

where $\hbar = h/2\pi$ is the Dirac's constant, k_B is the Boltzmann constant, and g_c 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_c-values, calculated using Equation (5), are given as follows.

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

(ii) If $g_c = 5$, one then obtains: $n_i = 9.77 \times 10^9\ cm^{-3}$, 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 $g_c = 4.9113$, one then gets: $n_i = 9.68 \times 10^9\ cm^{-3}$, according to a result proposed by Couderc et al. (C) as [38]: $n_{i(C)} = 1.541 \times 10^{15} \times T^{1.721} \times \exp\left(-\frac{E_{gi}}{2kT}\right)\ cm^{-3} = 9.68 \times 10^9\ cm^{-3}$ for T=300 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 Equation (5) and in donor-Si systems, the numerical results of n_i, calculated for $g_c = 6$, as a function of T, are plotted in Figure 1. Then, those of n_i, calculated for $g_c = 6, 5,$ and 4.9113 as functions of T, are tabulated in Table 2.

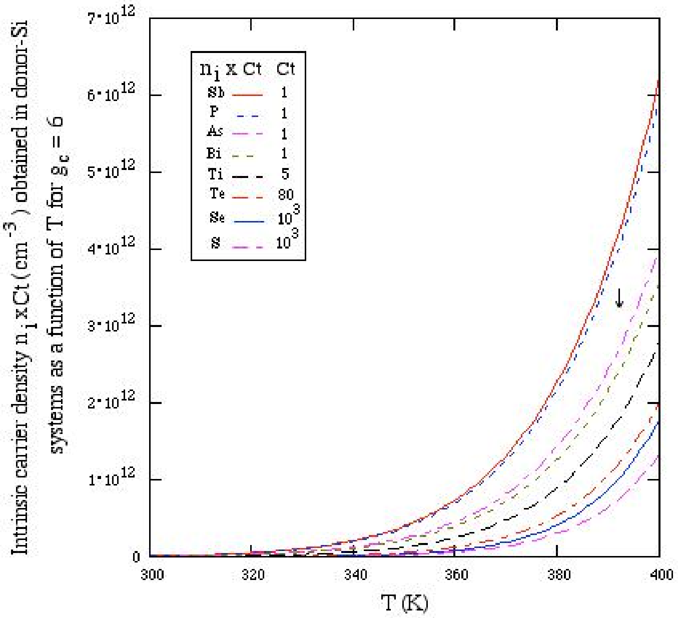


Figure 1. The intrinsic carrier density $n_i(T, r_d)$, plotted as functions of T, increases with increasing T for a given r_d, and decreases (↓) with increasing r_d for a given T, due to the donor-size effect.

Table 2. The values of intrinsic carrier concentration $n_i(T, r_{d(a)}, g_c)$ and intrinsic band gap E_{gi} are calculated for $g_c = 6, 5,$ and 4.9113, using Equations (5, 2), respectively, as functions of T and $r_{d(a)}$.

Donor	*Sb*	*P*	*As*	*Bi*	*Ti*	*Te*	*Se*	*S*

				$g_c = 6$				
$E_{gi}(300K)$ in eV	1.1215	1.1245	1.1515	1.1595	1.2875	1.5015	1.6835	1.7035
$n_i(300K)$ in $10^{10}\ cm^{-3}$	1.13	1.07	6.34×10^{-1}	5.43×10^{-1}	4.56×10^{-2}	7.26×10^{-4}	2.14×10^{-5}	1.46×10^{-5}
$n_i(350K)$ in $10^{11}\ cm^{-3}$	4.08	3.88	2.48	2.17	2.59×10^{-1}	7.44×10^{-3}	3.64×10^{-4}	2.61×10^{-4}
$n_i(400K)$ in $10^{12}\ cm^{-3}$	6.22	5.96	4.02	3.58	5.58×10^{-1}	2.49×10^{-2}	1.77×10^{-3}	1.33×10^{-3}
$n_i(450K)$ in $10^{13}\ cm^{-3}$	5.34	5.13	3.62	3.26	6.24×10^{-1}	3.94×10^{-2}	3.76×10^{-3}	2.90×10^{-3}
				$g_c = 5$				
$n_i(300K)$ in $10^{10}\ cm^{-3}$	1.04	9.77×10^{-1}	5.79×10^{-1}	4.96×10^{-1}	4.17×10^{-2}	6.63×10^{-4}	1.96×10^{-5}	1.33×10^{-5}
$n_i(350K)$ in $10^{11}\ cm^{-3}$	3.72	3.54	2.26	1.98	2.37×10^{-1}	6.80×10^{-3}	3.32×10^{-4}	2.38×10^{-4}
$n_i(400K)$ in $10^{12}\ cm^{-3}$	5.68	5.44	3.67	3.27	5.09×10^{-1}	2.28×10^{-2}	1.62×10^{-3}	121×10^{-3}
$n_i(450K)$ in $10^{13}\ cm^{-3}$	4.87	4.68	3.30	2.98	5.70×10^{-1}	3.59×10^{-2}	3.43×10^{-3}	2.65×10^{-3}
				$g_c = 4.9113$				
$n_i(300K)$ in $10^{10}\ cm^{-3}$	1.03	9.68×10^{-1}	5.74×10^{-1}	4.92×10^{-1}	4.13×10^{-2}	6.57×10^{-4}	1.94×10^{-5}	1.32×10^{-5}
$n_i(350K)$ in $10^{11}\ cm^{-3}$	3.69	3.51	2.24	1.96	2.35×10^{-1}	6.74×10^{-3}	3.29×10^{-4}	2.36×10^{-4}
$n_i(400K)$ in $10^{12}\ cm^{-3}$	5.63	5.39	3.64	3.24	5.05×10^{-1}	2.26×10^{-2}	1.61×10^{-3}	1.20×10^{-3}
$n_i(450K)$ in $10^{13}\ cm^{-3}$	4.83	4.64	3.28	2.95	5.65×10^{-1}	3.56×10^{-2}	3.40×10^{-3}	2.62×10^{-3}

Acceptor	***B***	***Al***	***Ga***	***In***	***Tl***
			$g_c = 6$		
$E_{gi}(300K)$ in eV	1.1245	1.1495	1.1555	1.2465	1.3415

$n_i(300\text{ K})$ in 10^{10} cm^{-3}	1.07	6.59×10^{-1}	5.87×10^{-1}	1.01×10^{-1}	1.60×10^{-2}

From those results, one remarks that: (i) n_i increases with increasing T for given r_d, and (ii) for T=300 K, for example, n_i decreases with increasing $r_{d(a)}$ since $E_{gi}(T,r_{d(a)})$ increases as observed in this Table 2, being due to the donor (acceptor)-size effect.

2.3. Heavy doping effect

First of all, in the donor-Si system, we define the effective intrinsic carrier concentration n_{ie}, by

$$n_{ie}^2 \equiv N \times p_o \equiv n_i^2 \times \exp\left[\frac{\Delta E_{ga}}{k_B T}\right] \qquad (8)$$

where n_i^2 is determined in Equation (5). Here, we can also define the "effective doping density" by [8]: $N_{Deff.} \equiv N/\exp\left[\frac{\Delta E_{ga}}{k_B T}\right]$ so that $N_{Deff.} \times p_o \equiv n_i^2$.

Here, p_o is the density of minority holes at the thermal equilibrium and the ABGN is defined by:

$$\Delta E_{ga} \equiv \Delta E_g + k_B T \times \ln\left(\frac{N}{N_C}\right) - E_F \qquad (9)$$

where N_C is defined in Equation (6), the Fermi energy E_F due to the effects of heavy doping and Fermi-Dirac statistics is determined in Equation (A3) of the Appendix A, being accurate within 2.11×10^{-4} [39], and the BGN, ΔE_g, due to the heavy doping effect, is determined in Equation (A15) of the Appendix B.

Furthermore, in order to determine the minority-carrier saturation current J_{Eo}, injected into the uniformly and heavily doped emitter region of the silicon devices, Jain and Roulston (JR) [15], Klaassen, Slotboom and Graaff (KSG) [16], Zouari and Arab (ZA) [17], Stem and Cid (SC) [18], and Yan and Cuevas (YC) [19], proposed their empirical expressions for the ABGN, being obtained in the P-Si system at 300 K, by:

$$\Delta E_{ga(JR)}(N) = 8.5\times10^{-3} \times\left\{\ln\left(\frac{N}{3.5\times10^{17}\text{ cm}^{-3}}\right) + \sqrt{\left[\ln\left(\frac{N}{3.5\times10^{17}\text{ cm}^{-3}}\right)\right]^2 + 0.5}\right\}\ (\text{eV}) \qquad (10)$$

$$\Delta E_{ga(KSG)}(N) = 6.92 \times 10^{-3} \times \left\{ \ln\left(\frac{N}{1.3 \times 10^{17}\ cm^{-3}}\right) + \sqrt{\left[\ln\left(\frac{N}{1.3 \times 10^{17}\ cm^{-3}}\right)\right]^2 + 0.5} \right\}\ (eV) \quad (11)$$

$$\Delta E_{ga(ZA)}(N) = 18.7 \times 10^{-3} \times \ln\left(\frac{N}{7 \times 10^{17}\ cm^{-3}}\right)\ (eV) \quad (12)$$

$$\Delta E_{ga(SC)}(N) = 14 \times 10^{-3} \times \ln\left(\frac{N}{1.4 \times 10^{17}\ cm^{-3}}\right)\ (eV) \quad (13)$$

$$\Delta E_{ga(YC)}(N) = 4.2 \times 10^{-5} \times \left[\ln\left(\frac{N}{10^{14}\ cm^{-3}}\right)\right]^3\ (eV) \quad (14)$$

Then, in such the P-Si system at 300K, being inspired by the term: $k_B T \times \ln\left(\frac{N}{N_C}\right)$ given in Equation (9), and also by the result: $\Delta E_{ga(YC)}(N)$ given in Equation (14), we can now propose a modified (Mod.) YC-model for the ABGN so that its numerical results are found to be closed to those calculated by using Equation (9), as:

$$\Delta E_{ga(Mod.YC)}(N, g_c) = 114.94 \times 10^{-6} \times \left[\ln\left(\frac{5.7167 \times 10^3}{N_C} \times \frac{N \times 6}{g_c}\right)\right]^3\ (eV) = 114.94 \times 10^{-6} \times \left[\ln\left(\frac{N \times \left(\frac{6}{g_c}\right)}{5 \times 10^{15}\ cm^{-3}}\right)\right]^3 (eV) \quad (15)$$

having a same empirical form as that given in Equation (14).

Now, for $g_c = 6$, in d-Si systems at 300 K, our numerical ABGN (ΔE_{ga})-results are calculated, using Equation (9). First, ours, obtained in the P-Si system, are plotted as a function of N in Figure 2 (a), in which the other ones, calculated using Equations (10-15), are also included, for a comparison. Secondly, in the P-Si system, the relative deviations between ours and the others are also plotted as functions of N in Figure 2 (b). Finally, in Figure 2 (c_1, c_2), ours are plotted in donor-Si systems as a function of N.

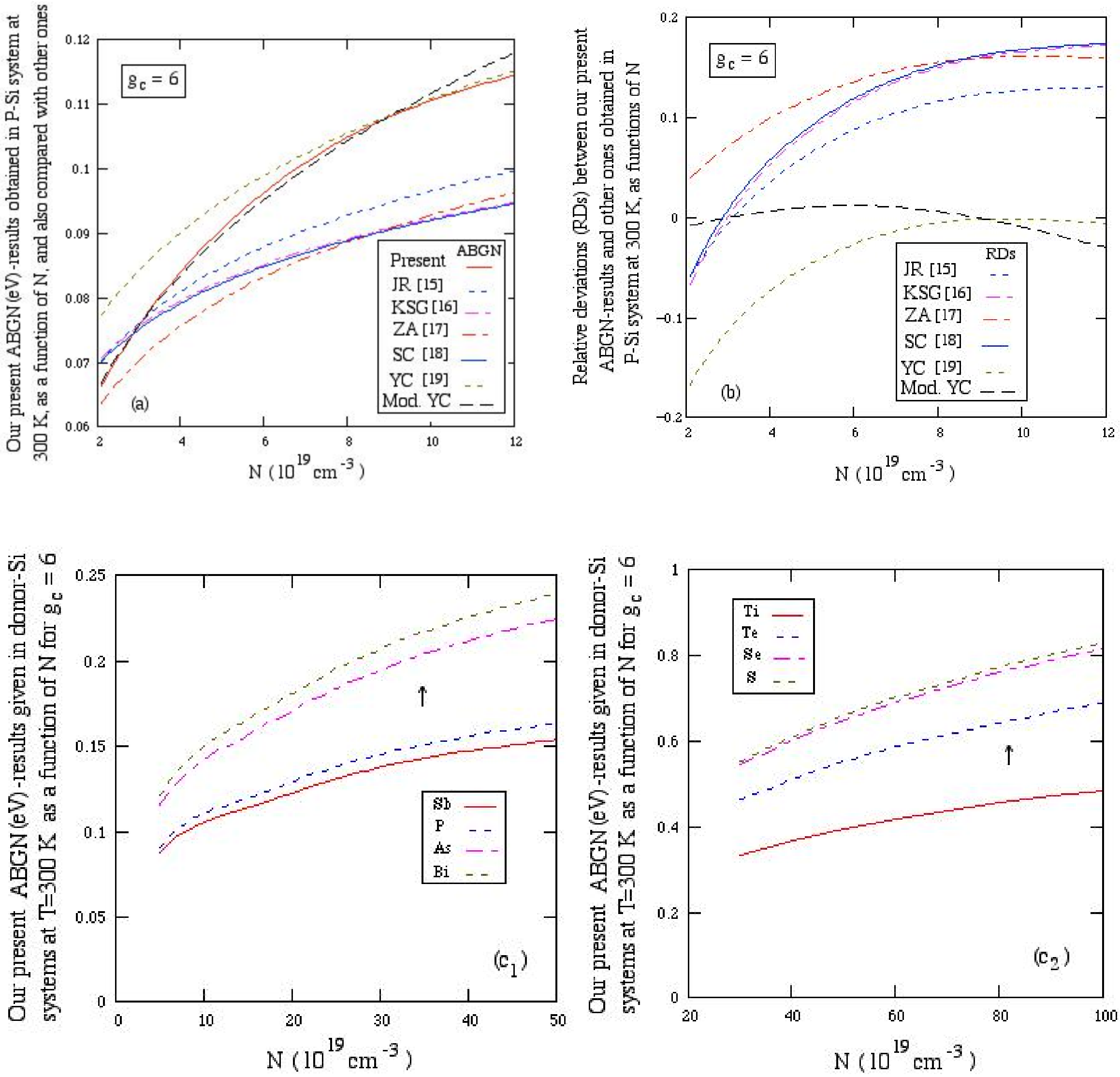


Figure 2. (a) Comparison of ABGN (ΔE_{ga})-results given in the P-Si system, (b) comparison of relative ABGN-deviations given in the P-Si system, and (c_1, c_2) our ABGN-results given in heavily doped donor-Si systems, with a condition: $N > N_{cn}(r_d)$, as that given in Table 1.

Here, one observes that:

(i) ours and our numerical ABGN-results obtained using Equation (15) are found to be closed together as seen in Figure 2 (a), and their absolute maximal relative deviation yields: 3.03%, which occurs at $N = 1.2 \times 10^{20}\ \text{cm}^{-3}$, as observed in Figure 2 (b), and

(ii) in Figure 2 (c_1, c_2), for a given donor-Si system, due to the heavy doping effect, ours increase with increasing N, and for a given N, due to the donor-size effect, ours increase (↑) with increasing r_d.

Moreover, it should be noted that our ABGN-expression (9) and other ones (10-15), given in the P-Si system at 300K, may be differently varied as functions of high N, as seen in Figure 2 (a).

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]:

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

where the intrinsic band gap E_{gi} is determined in Equation (2), the BGN ΔE_g is investigated in Equation (A15) 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}.

Now, in donor-Si systems, our present OBG-results, calculated using Equation (16) for $g_c = 6$ and T=300 K are plotted as functions of N in the following Figure 3.

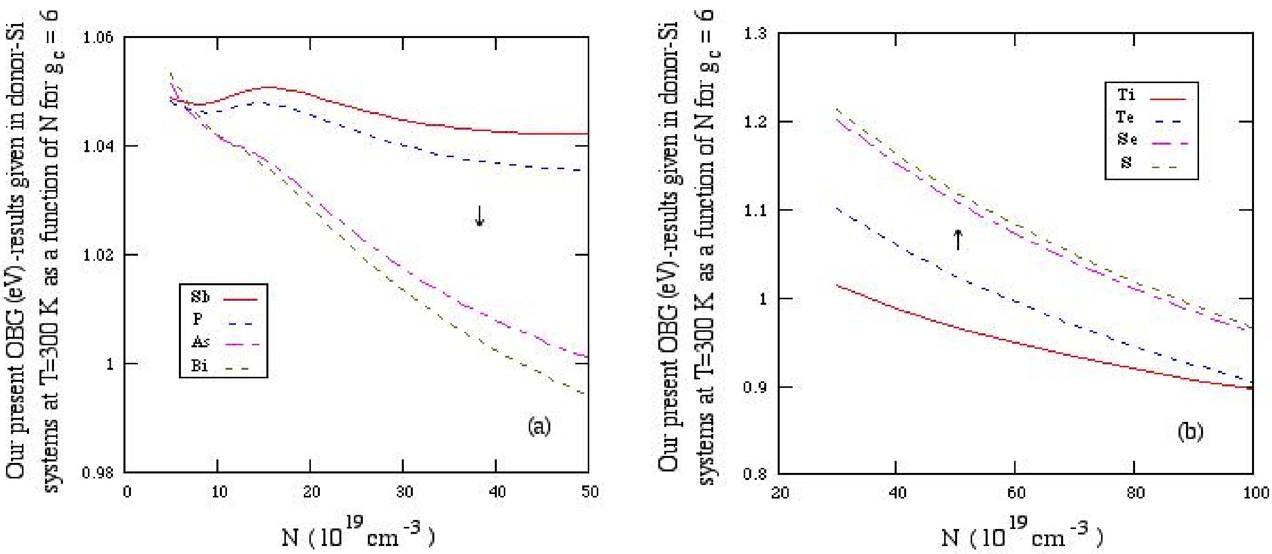


Figure 3. For $N > N_{cn}(r_d)$, our OBG (E_{g1})-results, (a) and (b), obtained in donor-systems, and plotted as functions of N.

Here, one observes that:

(i) with increasing r_d and for a given N, due to the donor-size effect, in (Sb, P, As, Bi)-Si systems the OBG decreases (↓), as given in Figure (a), while in (Ti, Te, Se, S)-Si systems it increases (↑), as seen in Figure (b), and

(ii) in a given donor-Si system and at $N \geq 3 \times 10^{20}\ cm^{-3}$, due to the heavy doping effect, the OBG decreases with increasing N, as seen in Figures (a) and (b), suggesting that from Equation (16) **the BGN-effect is found to be more important than the Fermi-energy one**.

Furthermore, it is possible to establish a conjunction between the electrical and optical phenomena, obtained from Equations (9, 16), by:

$$E_{g1}(N,T,r_d,g_c) \equiv E_{gi}(T,r_d) - \Delta E_{ga}(N,T,r_d,g_c) + k_B T \times \ln\left(\frac{N}{N_C(T,r_d,g_c)}\right)$$

which can be rewritten, for example, replacing ΔE_{ga} by $\Delta E_{ga(Mod.YC)}(N)$ determined in Equation (15), as:

$$E_{g1(Mod.YC)}(N,T,r_d,g_c) \equiv E_{gi}(T,r_d) - \Delta E_{ga(Mod.YC)}(N,g_c) + k_B T \times \ln\left(\frac{N}{N_C(T,r_d,g_c)}\right) \quad (17)$$

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} and $E_{g1(Mod.YC)}$, obtained for $g_c = 6$, are accurate within 1.86% and 1.9%, respectively, and found to thus 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: $1 - \frac{\text{Calculated } E_{g1}-\text{results}}{E_{g1}-\text{data}}$.

Table 3. Our numerical results of optical band gap (OBG), expressed as functions of N for $g_c = 6, 5, 4.9113$, and their relative deviations.

$N\ (10^{18}\ cm^{-3})$	4	8.5	15	50	80	150
E_{g1}(eV)-data [44]	1.020	1.028	1.033	1.050	1.056	1.059
Our OBG-results are obtained, using Equation (16).						
$g_c = 6$						
E_{g1}(eV)	1.0390	1.0465	1.0496	1.0483	1.0463	1.0479
RD(%)	-1.86	-1.80	-1.61	0.17	0.92	1.05
$g_c = 5$						

$E_{g1}(eV)$	1.0411	1.0478	1.0501	1.0473	1.0462	1.0470
RD(%)	<u>-2.07</u>	-1.92	-1.66	0.25	0.92	1.14
$g_c = 4.9113$						
$E_{g1}(eV)$	1.0413	1.0479	1.0502	1.0473	1.0463	1.0468
RD(%)	<u>-2.09</u>	-1.93	-1.66	0.26	0.92	1.15
Other OBG-results are obtained from Equation (17).						
$g_c = 6$						
$E_{g1(Mod.YC)}(eV)$	1.0394	1.0459	1.0489	1.0492	1.0469	1.0415
RD(%)	<u>-1.90</u>	-1.74	-1.54	0.08	0.86	1.66
$g_c = 5$						
$E_{g1(Mod.YC)}(eV)$	1.0412	1.0470	1.0495	1.0485	1.0456	1.0394
RD(%)	<u>-2.08</u>	-1.85	-1.59	015	0.98	1.85
$g_c = 4.9113$						
$E_{g1(Mod.YC)}(eV)$	1.0414	1.0471	1.0495	1.0484	1.0454	1.0392
RD(%)	<u>-2.09</u>	-1.86	-1.60	0.15	0.99	1.87

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

Here, our best choice is $g_c = 6$, meaning that at $T \geq 300$ K, due to the high thermal agitation energy $k_B T$, all the six equivalent conduction-band edges are effective.

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_{Eo}, injected into the heavily doped n-type emitter-region, we need to know an expression for the minority-hole mobility μ_h, being related to the minority-hole diffusion coefficient D_h, by the well-known

Einstein relation: $D_h = \frac{k_B T}{e} \times \mu_h$, 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:

$$\mu_h(N,T,r_d,g_c) = \left[130 + \frac{500-130}{1+\left(\frac{N\times 6}{8\times 10^{17}\ \mathrm{cm}^{-3}\times g_c}\right)^{1.25}}\right] \times \left(\frac{\varepsilon(r_d)}{\varepsilon(r_P)}\right)^2 \times \left(\frac{T}{300\ \mathrm{K}}\right)^{3/2} \quad (\mathrm{cm}^2\mathrm{V}^{-1}\mathrm{s}^{-1}) \tag{18}$$

noting that as T = 300 K, $g_c = 6$, and $r_d \equiv r_P$, Equation (18) is reduced to that investigated by del Alamo et al. [10]. Further, from Equations (5, 8, 9, 15, 18), we can define the following minority-hole transport parameter F as [8, 22, 25]:

$$F(N,T,r_d,g_c) \equiv \frac{n_i^2}{p_o \times D_h} = \frac{N_{Deff.}}{D_h} \equiv \frac{N}{D_h \times \exp\left[\frac{ABGN}{k_B T}\right]}\ (\mathrm{cm}^{-5}\times \mathrm{s}),\ N_{Deff.} \equiv \frac{N}{\exp\left[\frac{ABGN}{k_B T}\right]} \tag{19}$$

where $N_{Deff.}$ is the "effective doping density" [8] and the ABGN is determined in Equation (9) for our ΔE_{ga}-result or in Equation (15) for our approximate $\Delta E_{ga(Mod.YC)}$-one.

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

$$L_h^{-2}(N,T,r_d,g_c) = [\tau_h \times D_h]^{-1} = (C\times F)^2 = \left(C\times \frac{N_{Deff.}}{D_h}\right)^2 = \left(C\times \frac{n_i^2}{p_o \times D_h}\right)^2 \tag{20}$$

where the constant $C[= 10^{-17}\ (\mathrm{cm}^4/\mathrm{s})]$ was chosen in this work. Here, one remarks that τ_h can be computed since D_h (or μ_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]:

$$J_{Bo}(N_a,T,r_a) = \frac{e\times n_i^2(T,r_a,g_c=6)\times \sqrt{\frac{D_e(N_a,T,r_a)}{\tau_e(N_a)}}}{N_a} \tag{21}$$

where $n_i^2(T, r_{d(a)}, g_c = 6)$ is determined in Equation (5) and $D_e(N_a, T, r_a) \equiv \frac{k_B T}{e} \times \mu_e(N_a, T, r_a)$ 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, μ_e is the minority-electron mobility, being determined by [3, 11, 16]:

$$\mu_e(N_a, T, r_a) = \left[92 + \frac{1360 - 92}{1 + \left(\frac{N_a}{1.3 \times 10^{17}\text{cm}^{-3}}\right)^{0.91}}\right] \times \left(\frac{\varepsilon(r_a)}{\varepsilon(r_B)}\right)^2 \times \left(\frac{T}{300\ \text{K}}\right)^{3/2} \ (\text{cm}^2\text{V}^{-1}\text{s}^{-1}) \tag{22}$$

being reduced to the result obtained by Slotbottom and de Graaff [3, 16], as T=300 K and $r_a = r_B$, and $\tau_e(N_a)$ is the minority-electron lifetime, computed by [16, 25]:

$$\tau_e(N_a)^{-1} = \frac{1}{2.5 \times 10^{-3}} + 3 \times 10^{-13} \times N_a + 1.83 \times 10^{-31} \times N_a^2. \tag{23}$$

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.

Now, in d(a)-Si systems at 300 K and for $g_c = 6$, using Equations (18, 22), our numerical results of $\mu_{h(e)}$ are plotted as functions of N (N_a) in Figures 4 (a_1,a_2), (b). Then, these results indicate that:

(i) for given N (N_a), they decrease (↓) with increasing $r_{d(a)}$, due to the impurity-size effect, being in good accordance with that obtained in the d-Si system by Logan et al. [9], as: $\mu(\text{Sb}) > \mu(P) > \mu(As)$, and

(ii) for given $r_{d(a)}$, they slightly decrease with increasing N (N_a).

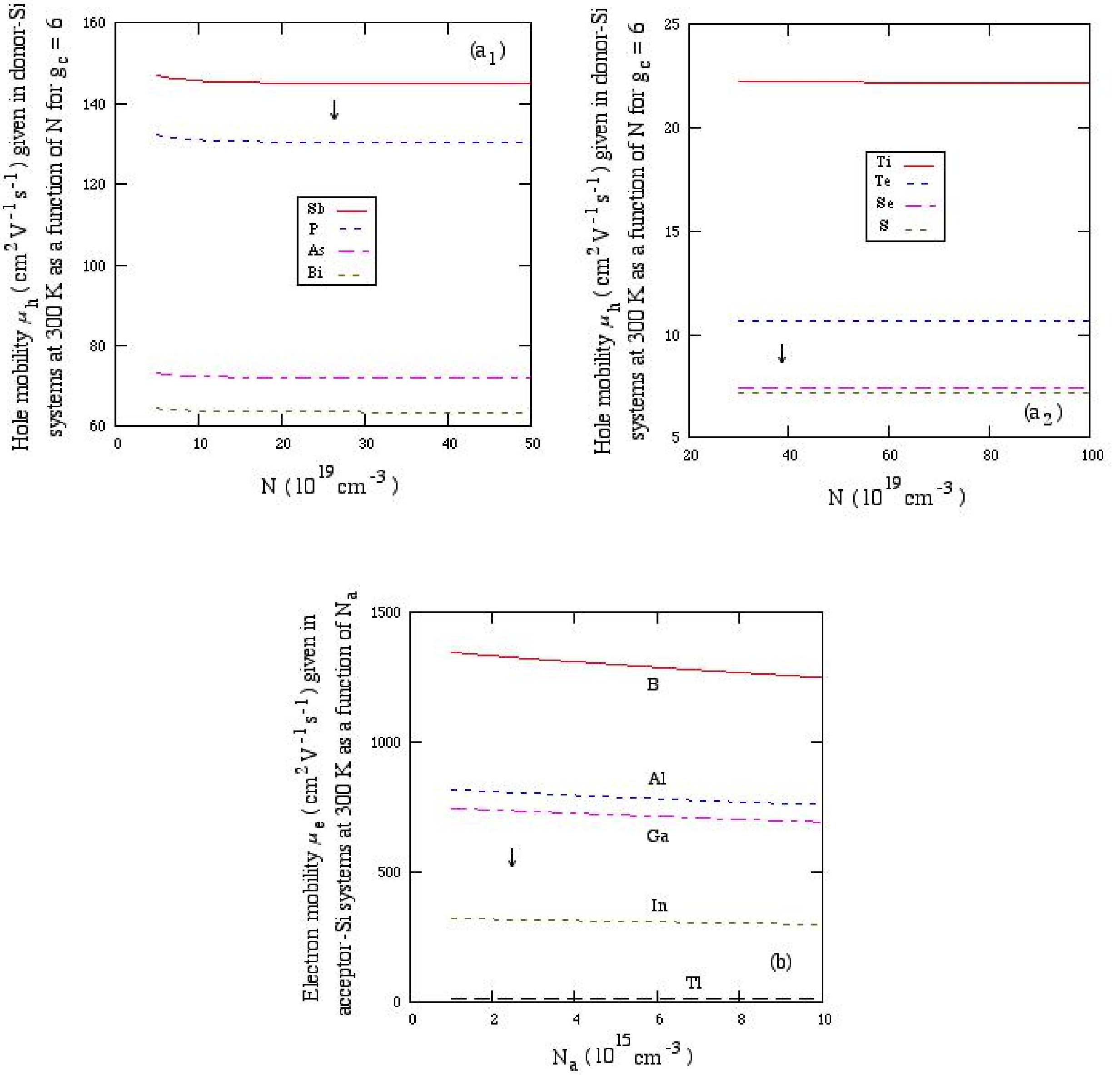


Figure 4. (a_1,a_2) Our μ_h-results given in heavily doped donor-Si systems, and (b) our μ_e-results given in lightly doped acceptor-Si systems, are respectively plotted as functions of N (N_a).

In the following, we will determine the minority-hole saturation-current density J_{Eo}, injected into the heavily doped n-type emitter-region of the $n^+ - p$ 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-region width W, by:

$$\rho(x) = N \times \exp\left\{-\left(\frac{x}{W}\right)^2 \times \ln\left[\frac{N}{N_o(W)}\right]\right\} \equiv N \times \left[\frac{N}{N_o(W)}\right]^{-\left(\frac{x}{W}\right)^2} \quad (24)$$

where $N_o(W) \equiv 7.9 \times 10^{17} \times \exp\left\{-\left(\frac{W}{0.1842\ \mu m}\right)^{1.066}\right\}\ (cm^{-3})$, $1\ \mu m = 10^{-4}\ cm$, 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, $\rho(W) = N_o(W)$, which decreases with increasing W, as noted above. Here, we also remark that $N_{o(VCD)} = 7 \times 10^{17}\ cm^{-3}$ was proposed by Van Cong and Debiais (VCD) [22], and $N_{o(ZA)} = 2 \times 10^{16}\ cm^{-3}$, 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_{Eo}–values are minimized, as seen in next Table 4, and our numerical calculation indicates that, from Equation (24), we can determine the highest value of W, being equal here to 85 µm. ww

Now, from Equations (8, 9) or Equation (19), taken for $0 \leq x \leq W$, and using Equation (24), the result: $N_{Deff.}(x = 0) \equiv N/\exp\left[\frac{\Delta E_{ga}(N)}{k_B T}\right]$ may be rewritten as:

$$N_{Deff.}(x) \equiv \rho(x)/\exp\left[\frac{\Delta E_{ga}(\rho(x))}{k_B T}\right] \quad (25)$$

which gives at x=W: $N_{Deff.}(W) \equiv \frac{N_o(W)}{\exp\left[\frac{\Delta E_{ga}(N_o(W))}{k_B T}\right]}$.

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:

$$p_o(x) \equiv \frac{n_i^2}{N_{Deff.}(x)} \quad (26)$$

and a normalized excess minority-hole density [or a relative deviation between $p(x)$ and $p_o(x)$] by [22, 25]:

$$u(x) \equiv \frac{p(x) - p_o(x)}{p_o(x)} \quad (27)$$

which must verify the two following boundary conditions proposed by Shockley as [2]:

$$u(x=0) \equiv \frac{-J_h(x=0)}{eS \times p_o(x=0)} \tag{28}$$

$$u(x=W) \simeq \exp\left(\frac{V}{n(V) \times V_T}\right) - 1, \text{ for small W} - \text{values} \tag{29}$$

Here, $n(V)$ is an ideality factor, $S\,(\frac{cm}{s})$ 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]:

$$J_h(x) = -\frac{en_i^2}{F(x)} \times \frac{du(x)}{dx} = -\frac{en_i^2 D_h(x)}{N_{Deff.}(x)} \times \frac{du(x)}{dx} \tag{30}$$

where $F(x)$ is determined in Equation (19), in which N is replaced by $\rho(x)$, proposed in Equation (24).

Further, the minority-hole continuity equation yields [8, 22]:

$$\frac{dJ_h(x)}{dx} = -en_i^2 \times \frac{u(x)}{F(x) \times L_h^2} = -en_i^2 \times \frac{u(x)}{N_{Deff.}(x) \times \tau_h(\rho(x))} = -e \times [p(x) - p_0(x)] \times \frac{\tau_h(N)}{\tau_h(\rho(x))} \times \frac{1}{\tau_h(N)} \tag{31}$$

.

Then, from these two Equations (30, 31), one obtains the following second-order differential equation as [22]:

$$\frac{d^2u(x)}{dx^2} - \frac{dF(x)}{dx} \times \frac{du(x)}{dx} - \frac{u(x)}{L_h^2(x)} = 0 \tag{32}$$

Using the two boundary conditions (28, 29), one thus gets the general solution of this Equation (32) as [22]:

$$u(x) = [A(W) \times \sinh(P(x)) + B(W) \times \cosh(P(x))] \times \left(\exp\left(\frac{V}{n(V) \times V_T}\right) - 1\right) \tag{33}$$

where $A(W) \equiv \frac{1}{\sinh(P(W)) + I(W) \times \cosh(P(W))}$, $I(W,S) \equiv \frac{B}{A} = \frac{D_h(N_o(W))}{S \times L_h(N_o(W))}$ and $P(x) \equiv \int_0^x C \times F(x)dx$, since $\frac{dP(x)}{dx} \equiv C \times F(x)$. Here, $C = 10^{-17}\ (cm^4/s)$, as that chosen in Equation (20), and the hyperbolic sine-and-cosine functions are defined by: $\sinh(x) \equiv 0.5 \times [e^x - e^{-x}]$ and $\cosh(x) \equiv 0.5 \times [e^x + e^{-x}]$.

Further, from Eq. (33), as $P(W) \ll 1$ (or for small W) one has: $A \simeq \frac{1}{I}$ or $B \simeq 1$, and one therefore obtains: $u(W) \simeq \left[\exp\left(\frac{V}{n(V)\times V_T}\right) - 1\right]$, which is just the boundary condition given in Equation (29).

Now, using Equations (30, 33), one gets:

$$J_h(x, N, T, r_d, g_c, S) = -J_{Eo}(x, N, T, r_d, g_c, S) \times \left(\exp\left(\frac{V}{n(V)\times V_T}\right) - 1\right) \tag{34}$$

where J_{Eo} is the minority-hole saturation current density, being injected into the heavily doped n-type emitter region for $0 \le x \le W$ and given by:

$$J_{Eo}(x, N, T, r_d, g_c, S) = en_i^2 C \times [A(W) \times \cosh(P(x)) + B(W) \times \sinh(P(x))] \tag{35}$$

One also remarks that, from Equations (20, 33-35) and after some manipulations, one gets: $u(x = 0) \equiv \frac{-J_h(x=0)}{eS\times p_o(x=0)}$, 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 effective minority-hole diffusion length by:

$$\frac{1}{L_{h,eff.}(x = W, N, T, r_d, g_c)} = \frac{1}{W}\int_0^W \frac{dx}{L_h(x)} = \frac{1}{W}\int_0^W C \times F(x)dx \equiv P(x = W, N, T, r_d, g_c)/W \tag{36}$$

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

$$P(x = W, N, r_d, g_c) \equiv \frac{W}{L_{h,eff.}} = \frac{W}{L_h} \times \frac{L_h}{L_{h,eff.}} \tag{37}$$

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

$$J_{Eo}(x = 0, N, r_d, g_c, S) = en_i^2 C \times A = \frac{en_i^2 C}{\sinh(P) + I \times \cosh(P)} \tag{38}$$

$$J_{Eo}(x = W, N, r_d, g_c, S) = en_i^2 C \times \frac{\cosh(P) + I \times \sinh(P)}{\sinh(P) + I \times \cosh(P)} \tag{39}$$

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

$$\frac{J_h(x = 0, N, r_d, g_c, S)}{J_h(x = W, N, r_d, g_c, S)} \equiv \frac{J_{Eo}(x = 0, N, r_d, g_c, S)}{J_{Eo}(x = W, N, r_d, g_c, S)} = \frac{1}{\cosh(P) + I \times \sinh(P)} \tag{40}$$

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

$\frac{1}{J_{Eo}(x=W)} \times \left[J_{Eo}(x=W) - J_{Eo}(x=0) = \frac{1}{\tau_h(N)} \times Q_{h,\,eff.}(x=W,N)\right]$,
(41)

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

$$Q_{h,\,eff.}(x=W,N) \equiv \int_0^W e \times [p(x) - p_0(x)] \times \frac{\tau_h(N)}{\tau_h(\rho(x))} dx. \quad (42)$$

Finally, from Equations (40, 41), if defining the effective minority-hole transit time by: $\tau_{t,eff.}(x=W,N,S) \equiv Q_{h,\,eff.}(x=W,N)/J_{Eo}(x=W,N,r_d,g_c,S)$, one then obtains the reduced effective minority-hole transit time, as:[22]

$$\frac{\tau_{t,eff.}(x=W,N,r_d,g_c,S)}{\tau_h} = 1 - \frac{J_{Eo}(x=0,N,r_d,g_c,S)}{J_{Eo}(x=W,N,r_d,g_c,S)} = 1 - \frac{1}{\cosh(P) + I \times \sinh(P)}. \quad (43)$$

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

5.1. Very large $S(=10^{50}\ \frac{cm}{s},\ for\ example)$ or $S \to \infty$ and $P \ll 1$ or $W \ll L_{h,eff.}$

Here, various results can be investigated as follows.

(i) From Equations (38-40), since $I(W) = \frac{D_h(N_o(W))}{S \times L_h(N_o(W))} \to 0$ as $S \to \infty$, $\frac{J_{Eo}(x=0,N,r_d,g_c,S)}{J_{Eo}(x=W,N,r_d,g_c,S)} \simeq \frac{1}{\cosh(P)} \to 1$ since $P \ll 1$, or $J_{Eo}(x=W,N,r_d,g_c,S\to\infty) \simeq J_{Eo}(x=0,N,r_d,g_c,S\to\infty)$. Therefore, from

Equation (43), one obtains: $\frac{\tau_{t,eff.}(x=W,N,r_d,g_c,S\to\infty)}{\tau_h(N)} \to 0$, suggesting a completely transparent emitter

region (CTER).

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

$$J_{Eo}(x=W,N,r_d,g_c,S\to\infty) \simeq \frac{en_i^2 C}{P} = \frac{en_i^2}{F \times W} \times \frac{L_{h,eff.}}{L_h} = \frac{en_i^2 \times D_h \times \exp\left[\frac{ABGN}{k_B T}\right]}{N \times W} \times \frac{L_{h,eff.}}{L_h} \quad (44)$$

being found to be independent of S and C, since $\frac{L_{h,eff.}}{L_h}$ 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).

Moreover, by a similar way, this result (44) can also be applied to calculate the electron-minority saturation current density as:

$$J_{Eo}(x = W, N_A, r_B, g_v, S \to \infty) \simeq \frac{en_i^2 \times D_e \times \exp\left[\frac{ABGN}{k_BT}\right]}{N \times W} \times \frac{L_{e,eff.}}{L_e} = \frac{en_i^2 \times D_e}{N_{Aeff} \times W} \times \frac{L_{e,eff.}}{L_e},\ N_{Aeff} \equiv \frac{N_A}{\exp\left[\frac{ABGN}{k_BT}\right]},$$

being injected into the heavily doped p-type doped emitter region of $p^+ - n$ junction. Then, Cuevas et al. (C) [21] used a simplified form as: $J_{Eo(C)} \simeq \frac{en_i^2 \times D_e}{N_{Aeff} \times W}$ to explain their experimental results obtained from the samples: 2B1, 2B2, 2B3, 2B4 and 2B5, as those given in Table 1 of this Reference 21, giving the relative deviations in absolute values equal to: 28.6%, 0%, 66.7%, 220% and 200%, respectively. It means that this simplified $J_{Eo(C)}$-formula is found to be inaccurate, due to the fact that they neglected an important ($\frac{L_{e,eff.}}{L_e}$)-effect, given in this heavily doped emitter region.

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 J_{Eo}-results are calculated, using Equations (44, 9) and (44, 15), and tabulated in Table 4, in which the CTER -condition, $P \ll 1$ (or $\frac{\tau_{t,eff.}}{\tau_h(N)} \ll 1$), is fulfilled, and we also compare them with modeling and measuring J_{Eo}-results investigated by del Alamo et al. (ASS) [10, 12]. One further notes that their modeling J_{Eo}-result [10] was based only on two independent parameters: N_{Deff}/D_h and L_h, as that obtained from our above result (44), for $L_{h,eff.} = W$. Therefore, this could explain a great difference between their modeling results [10, 12] accurate within 36%, and ours accurate within 1.78%, for $g_c = 6$, as observed in the following Table 4.

Table 4. Our present results of $J_{Eo}(S \to \infty)$ A/cm^2, expressed as functions of N for $g_c = 6, 5, 4.9113$, and their relative deviations (RDs), calculated by: RD(%)=1-(Present J_{Eo}/ J_{Eo}-data), where the J_{Eo}-data are given in References 10 and 12, and also the theoretical ASS- J_{Eo}-results, obtained by Alamo et al. (ASS) [10, 12], and their relative deviations.

$N\ (10^{19}\ cm^{-3})$	2.1	3.3	4.4	4.6	12
W (μm)	0.20	1.00	0.23	0.66	0.20
$J_{Eo}(S \to \infty)$–data	3.2×10^{-12}	8.3×10^{-13}	2.6×10^{-12}	1.1×10^{-12}	2.8×10^{-12}
ASS- $J_{Eo}(S \to \infty)$]	3.6×10^{-12}	1.1×10^{-12}	2.6×10^{-12}	1.5×10^{-12}	2.81×10^{-12}
RD(%)	-12.5	-32.5	0	-36	-0.4

$N_o(cm^{-3})$	2.65×10^{17}	1.82×10^{15}	2.22×10^{17}	1.60×10^{16}	2.65×10^{17}
Present J_{Eo}-results are obtained, using Equations (44, 9)					
$g_c = 6,\ n_i = 1.07 \times 10^{10}\ cm^{-3}$					
P(N, W)<<1	5.7×10^{-5}	2.2×10^{-4}	7.2×10^{-5}	1.7×10^{-4}	6.6×10^{-5}
$\frac{\tau_{t,eff.}}{\tau_h(N)} \ll 1$	1.6×10^{-9}	2.4×10^{-8}	2.6×10^{-9}	1.4×10^{-8}	2.2×10^{-9}
Present $J_{Eo}(S \to \infty)$	3.242×10^{-12}	8.448×10^{-13}	2.554×10^{-12}	1.080×10^{-12}	2.774×10^{-12}
RD(%)	-1.32	<u>-1.78</u>	1.77	<u>1.78</u>	0.94
$g_c = 5,\ n_i = 9.77 \times 10^{9}\ cm^{-3}$					
P(N, W)<<1	5.0×10^{-5}	1.9×10^{-4}	6.1×10^{-5}	1.4×10^{-4}	5.7×10^{-5}
$\frac{\tau_{t,eff.}}{\tau_h(N)} \ll 1$	1.2×10^{-9}	1.8×10^{-8}	1.9×10^{-9}	1.0×10^{-8}	1.6×10^{-9}
Present $J_{Eo}(S \to \infty)$	3.054×10^{-12}	8.124×10^{-13}	2.485×10^{-12}	1.052×10^{-12}	2.693×10^{-12}
RD(%)	<u>4.56</u>	2.12	4.43	4.35	3.81
$g_c = 4.9113,\ n_i = 9.68 \times 10^{9}\ cm^{-3}$					
P(N, W)<<1	4.9×10^{-5}	1.8×10^{-4}	6.1×10^{-5}	1.4×10^{-4}	5.6×10^{-5}
$\frac{\tau_{t,eff.}}{\tau_h(N)} \ll 1$	1.2×10^{-9}	1.7×10^{-8}	1.8×10^{-9}	1.0×10^{-8}	1.6×10^{-9}
J_{Eo} (A/cm^2)	3.038×10^{-12}	8.096×10^{-13}	2.479×10^{-12}	1.050×10^{-12}	2.686×10^{-12}
RD(%)	<u>5.07</u>	2.46	4.66	4.57	4.07
Present J_{Eo}-results are obtained, using Equations (44, 15)					
$g_c = 6,\ n_i = 1.07 \times 10^{10}\ cm^{-3}$					
P(N, W)<<1	5.7×10^{-5}	2.2×10^{-4}	7.2×10^{-5}	1.7×10^{-4}	6.5×10^{-5}
$\frac{\tau_{t,eff.}}{\tau_h(N)} \ll 1$	1.6×10^{-9}	2.3×10^{-8}	2.6×10^{-9}	1.5×10^{-8}	2.1×10^{-9}
Present $J_{Eo}(S \to \infty)$	3.277×10^{-12}	8.472×10^{-13}	2.543×10^{-12}	1.073×10^{-12}	2.813×10^{-12}
RD(%)	-2.41	-2.07	2.20	<u>2.42</u>	-0.48
$g_c = 5,\ n_i = 9.77 \times 10^{9}\ cm^{-3}$					

P(N, W)<<1	5.0×10^{-5}	1.9×10^{-4}	6.2×10^{-5}	1.5×10^{-4}	5.4×10^{-5}
$\frac{\tau_{t,eff.}}{\tau_h(N)} \ll 1$	1.2×10^{-9}	1.8×10^{-8}	1.9×10^{-9}	1.1×10^{-8}	1.5×10^{-9}
Present $J_{Eo}(S \to \infty)$	3.083×10^{-12}	8.107×10^{-13}	2.460×10^{-12}	1.040×10^{-12}	2.808×10^{-12}
RD(%)	3.66	2.32	5.37	<u>5.49</u>	-0.30
$g_c = 4.9113,\ n_i = 9.68 \times 10^9\ cm^{-3}$					
P(N, W)<<1	4.9×10^{-5}	1.9×10^{-4}	6.1×10^{-5}	1.4×10^{-4}	5.3×10^{-5}
$\frac{\tau_{t,eff.}}{\tau_h(N)} \ll 1$	1.2×10^{-9}	1.7×10^{-8}	1.9×10^{-9}	1.0×10^{-8}	1.4×10^{-9}
Present $J_{Eo}(S \to \infty)$	3.066×10^{-12}	8.075×10^{-13}	2.453×10^{-12}	1.037×10^{-12}	2.809×10^{-12}
RD(%)	4.20	2.71	5.64	<u>5.75</u>	-0.31

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

Table 4 indicates that:

- the maximal relative deviations (RDs) in absolute values between our results (44, 9) and the J_{Eo}-data [10, 12] are found to be: 1.78% for g_c=6, 4.56% for g_c=5, and 5.07% for g_c=4.9113, and

- the maximal RDs in absolute values between our results (44, 15) and the J_{Eo}-data [10, 12] are given by: 2.42% for g_c=6, 5.49% for g_c=5, and 5.75% for g_c=4.9113. It suggests that our numerical results (44, 9) for g_c=6 are the best ones, since they are accurate within 1.78%. Further, one notes that our ΔE_{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, while in Equation (15) our $\Delta E_{ga(Mod.YC)}$ -expression is only an empirical one. So, in the following, we will choose: g_c=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:

$$\frac{J_{Eo}(x=0,N,r_d,S)}{J_{Eo}(x=W,N,r_d,S)} = \frac{1}{\cosh(P)+I\times\sinh(P)} \simeq 1 - \frac{D_h(N_o(W))}{S\times L_h(N_o(W))} \times P - \frac{(P)^2}{2}.$$

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

$$\tau_{t,eff.}(x = W,N,r_d,g_c,S) \simeq \tau_h \times \left\{\frac{D_h(N_o(W))}{S \times L_h(N_o(W))} \times P + \frac{(P)^2}{2}\right\}$$
$$\simeq \frac{W}{S} \times \frac{L_h(N_o(W))}{L_{h,eff.}(N_o(W))} + \frac{W^2}{2D_h(N_o(W))} \times \left(\frac{L_h(N_o(W))}{L_{h,eff.}(N_o(W))}\right)^2 \quad (45)$$
$$\simeq \frac{W^2}{2D_h(N_o(W))} \times \left(\frac{L_h(N_o(W))}{L_{h,eff.}(N_o(W))}\right)^2, \text{ as } S \to \infty$$

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

$$\tau_{t,eff.}(x = W,N,r_d,S) \equiv \tau_t = \frac{W}{S} + \frac{W^2}{2D_h} \simeq \frac{W^2}{2D_h}, \text{ as } S \to \infty \quad (46)$$

being just a familiar expression given for the minority-hole transit time τ_t obtained by Shibib et al. [7].

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

Here, from Eq. (33) and for any N, one has: $I = \frac{D_h(N_o(W))}{S \times L_h(N_o(W))} \to \infty$, since $S \to 0$. Therefore, from Equation (43), one obtains: $\frac{\tau_{t,eff.}(x=W \gg \mathbf{L_{h,eff.}},N,r_d,g_c,S\to 0)}{\tau_h} \to 1$, suggesting a completely opaque emitter region (COER).

Now, our numerical results of $J_{Eo}(x = W, N,r_d,S) \equiv J_{Eo}$ and $\frac{\tau_{t,eff.}(x=W,N,r_d,S)}{\tau_h} \equiv \frac{\tau_{t,eff.}}{\tau_h}$, for simplicity, are respectively computed, using Equations (39) and (43), and then plotted into Figures 5 (a_1, a_2), (b) and 6 (a_1, a_2), (b), as a function of N, and Figures 5 (c) and 6 (c), as functions of S, noting that in those figures we also include various physical conditions such as: S, W, r_d and N, and in particular, due to the heavy doping effect, one must have: $N > N_{cn}(r_d)$, according to the heavily doped donor-Si systems, as those given in Table 1.

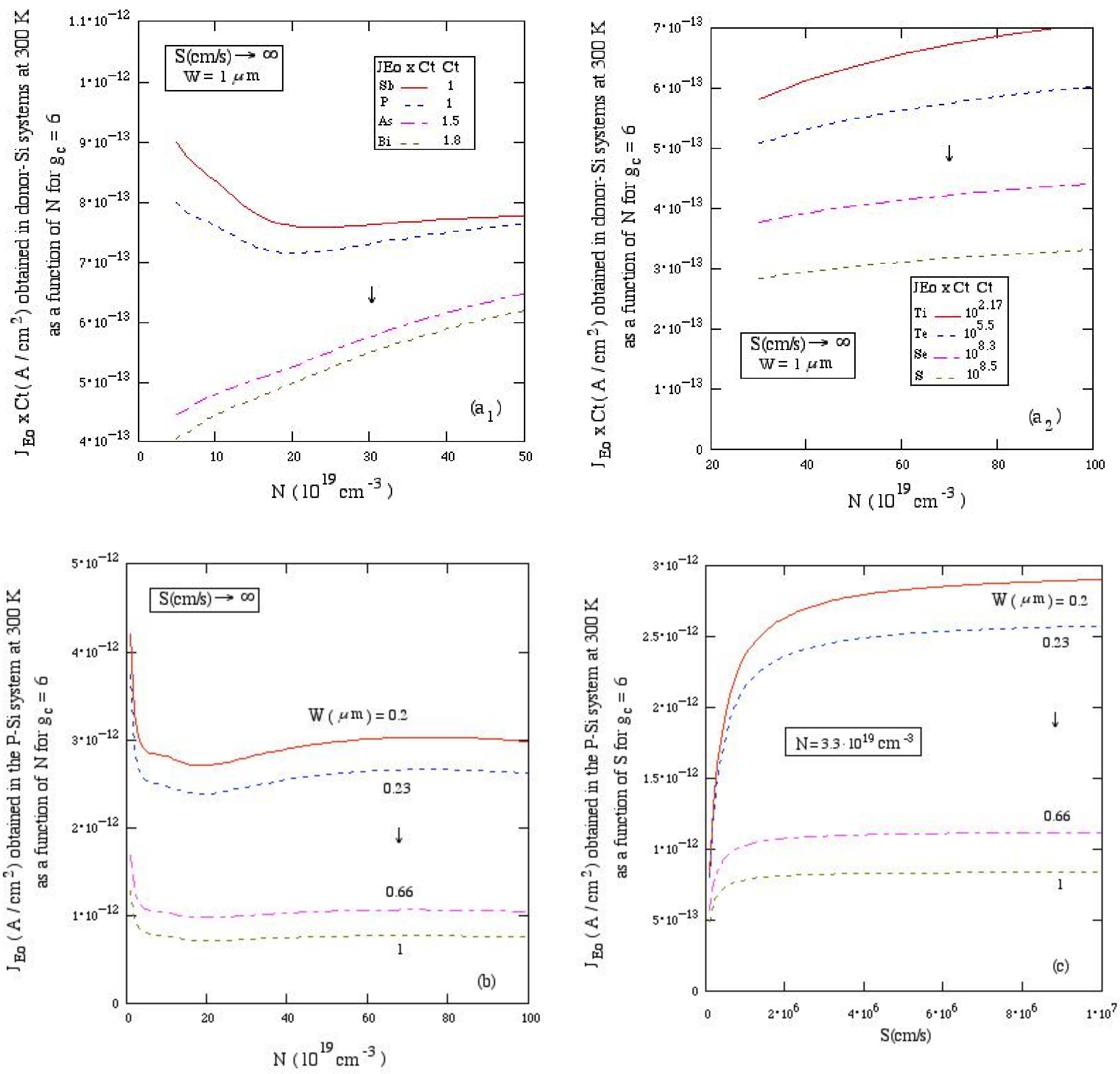


Figure 5. (a_1, a_2) Our J_{Eo}-results obtained as functions of N, with a condition: $N > N_{cn}(r_d)$, given in heavily doped donor-Si systems, as defined in Table 1, (b) our J_{Eo}-results obtained as functions of N in P-Si systems, and (c) our J_{Eo}-results obtained as functions of S in P-Si systems.

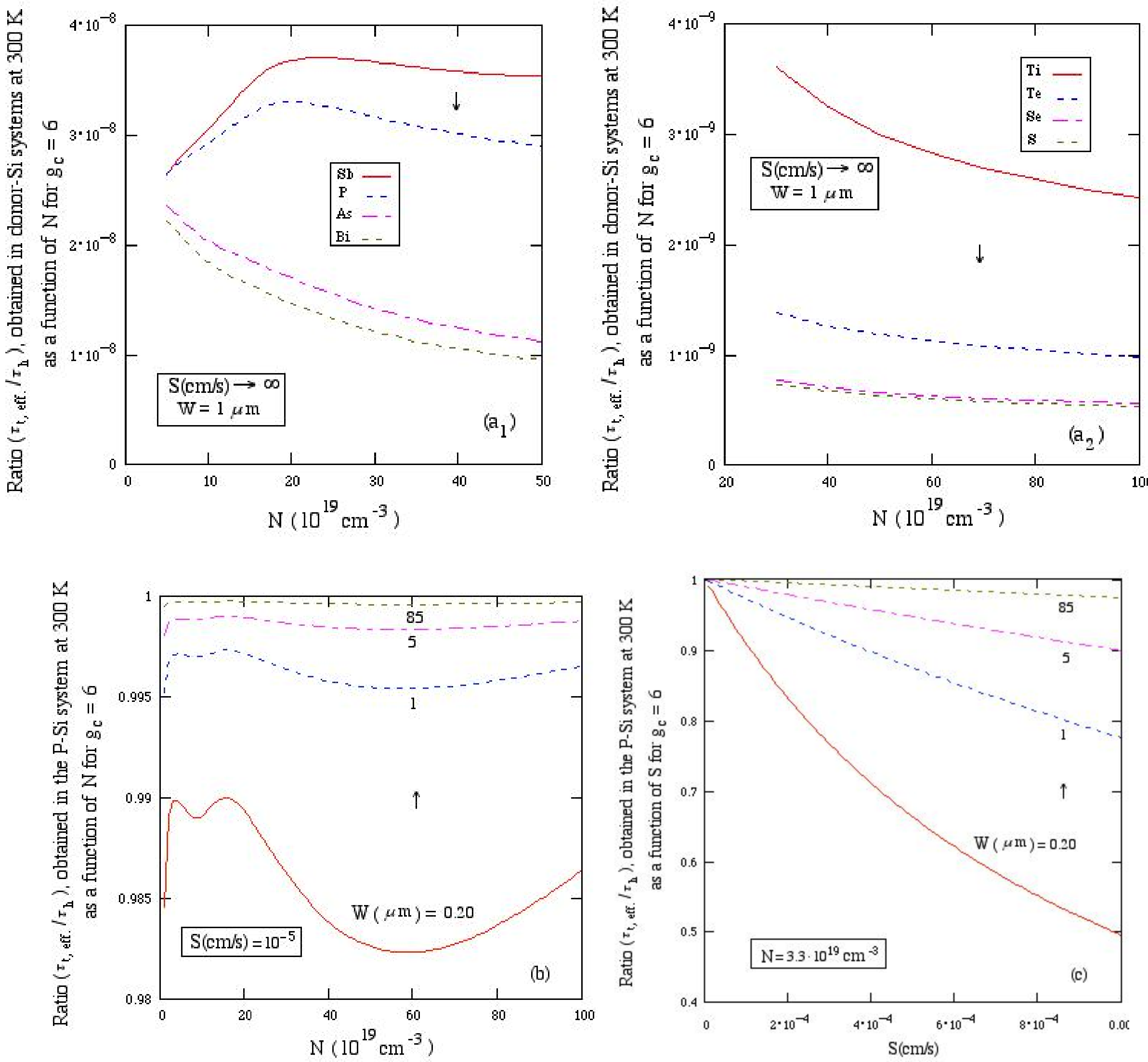


Figure 6.** **(a_1, a_2) Our ($\tau_{t,eff.}/\tau_h$)-results obtained as functions of $N > N_{cn}(r_d)$ in heavily doped donor-Si systems, as defined in Table 1, (b) our ($\tau_{t,eff.}/\tau_h$)-results obtained as functions of N in P-Si systems, and (c) our ($\tau_{t,eff.}/\tau_h$)-results obtained as functions of S in P-Si systems.

Some concluding remarks are obtained and discussed below.

(i) Figures 5(a_1, a_2) and 6(a_1, a_2) indicate that, since as $S \to \infty$ and $W = 1\ \mu m$, $\frac{\tau_{t,eff.}}{\tau_h}(< 4 \times 10^{-8}) \simeq 0$, according to the CTER, and for a given N, due to the donor-size eff**ect**, both J_{Eo} and $\frac{\tau_{t,eff.}}{\tau_h}$ decrease (↓) 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 $\frac{\tau_{t,eff.}}{\tau_h}$) increases (or decreases) with increasing N.

(ii) Figures 5(b) and 6(b) show that, for a given N, J_{Eo} (or $\frac{\tau_{t,eff.}}{\tau_h}$) decreases (or increases) with increasing W.

(iii) Figures 5(c) and 6(c), suggest that, for given S, J_{Eo} (or $\frac{\tau_{t,eff.}}{\tau_h}$) decreases (or increases) with increasing W.

(iv) In particular, in Figure 6(c), as $S \to 0$ and $W = 85\ \mu m$, $\frac{\tau_{t,eff.}}{\tau_h} \to 1$, 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:

$$J_o(x = W, N, r_d, S, N_a, r_a) \equiv J_{Eo}(x = W, N, r_d, S) + J_{Bo}(N_a, r_a) \tag{47}$$

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 $J_o = J_{Eo} + J_{Bo}$, calculated using Equation (47), where J_{Bo} and J_{Bo} are determined respectively in Equations (21, 39), and those are obtained in the three following cases.

First case: 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 $J_{Bo} = 6.0912 \times 10^{-13}\ \left(\frac{A}{cm^2}\right)$.

For $S = 10^{50}\ cm/s$ and $W = 0.206$ nm, according to the completely transparent emitter region, one has:

$J_{Eo} = 2.4833 \times 10^{-9}\ \left(\frac{A}{cm^2}\right) \gg J_{Bo}$ and $J_o = 2.4839 \times 10^{-9}\ \left(\frac{A}{cm^2}\right) \simeq J_{Eo}$

For $S = 10^{50}\ cm/s$ 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 $J_o = 1.1706 \times 10^{-10}\ \left(\frac{A}{cm^2}\right) \simeq J_{Eo}$

For $S = 10^4\ cm/s$ and $W = 0.36\ \mu m$, one has: $J_{Eo} = 1.2237 \times 10^{-13}\ \left(\frac{A}{cm^2}\right) < J_{Bo}$ and $J_o = 7.3148 \times 10^{-13}\ \left(\frac{A}{cm^2}\right) \simeq J_{Bo}$

For $S = 10^{-50}\ cm/s$ and $W = 85\ \mu m$, according also to the completely opaque emitter region, one has: $J_{Eo} = 4.7117 \times 10^{-19}\ \left(\frac{A}{cm^2}\right) \ll J_{Bo}$ and $J_o = 6.0912 \times 10^{-13}\ \left(\frac{A}{cm^2}\right) = J_{Bo}$

Second case: In the completely opaque HD S-Si emitter region ($N = 5 \times 10^{20}\ cm^{-3}$, $S = 10^{-50}\ cm/s$ and $W = 85\ \mu m$), and in the lightly doped a-Si base region, in which $N_a = 10^{16}\ cm^{-3}$.

(r_S, r_a)	(r_S, r_B)	(r_S, r_{Al})	(r_S, r_{Ga})	(r_S, r_{In})	(r_S, r_{Tl})
$J_{Eo}\ \left(\frac{A}{cm^2}\right)$	1.8728×10^{-29}	1.8728×10^{-29}	1.8728×10^{-29}	1.8728×10^{-29}	1.8728×10^{-29}
$J_{Bo}\ \left(\frac{A}{cm^2}\right)$	6.0912×10^{-13}	1.8033×10^{-13}	1.3660×10^{-13}	2.6485×10^{-15}	5.3080×10^{-17}

$J_o\left(\frac{A}{cm^2}\right)$	6.0912×10^{-13}	1.8033×10^{-13}	1.3660×10^{-13}	2.6485×10^{-15}	5.3080×10^{-17}

$J_o = J_{Bo}$

Third case: In the completely transparent HD d-Si emitter region ($N = 5 \times 10^{20}\ cm^{-3}$, $S = 10^{50}\ cm/s$ and $W = 0.000206\ \mu m$), and in the lightly doped Tl-Si base region, in which $N_a = 10^{16}\ cm^{-3}$ and $J_{Bo} = 5.3080 \times 10^{-17}\ \left(\frac{A}{cm^2}\right)$.

(r_d, r_{Tl})	(r_{Sb}, r_{Tl})	(r_P, r_{Tl})	(r_{As}, r_{Tl})	(r_{Bi}, r_{Tl})
$J_{Eo}\left(\frac{A}{cm^2}\right)$	2.7206×10^{-9}	2.6794×10^{-9}	1.5402×10^{-9}	1.2336×10^{-9}
$J_o\left(\frac{A}{cm^2}\right)$	2.7206×10^{-9}	2.6794×10^{-9}	1.5402×10^{-9}	1.2336×10^{-9}
(r_d, r_{Tl})	(r_{Ti}, r_{Tl})	(r_{Te}, r_{Tl})	(r_{Se}, r_{Tl})	(r_S, r_{Tl})
$J_{Eo}\left(\frac{A}{cm^2}\right)$	1.6600×10^{-11}	7.5378×10^{-15}	9.7654×10^{-18}	4.6878×10^{-18}
$J_o\left(\frac{A}{cm^2}\right)$	1.6600×10^{-11}	7.5909×10^{-15}	6.2845×10^{-17}	$5.7767 \times 10^{-17} \simeq J_{Bo}$

Some important remarks are given and discussed below.

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

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

(iii) In the third case or in the CTER-conditions, J_{Eo} decreases with increasing r_d, being due to the donor-size effect, and for (r_S, r_{Tl}), one gets: $J_o = 5.7767 \times 10^{-17}\ \left(\frac{A}{cm^2}\right) \simeq J_{Bo} = 5.3080 \times 10^{-17}\ \left(\frac{A}{cm^2}\right)$, which can be compared with the similar result, obtained the second case or in the COER-conditions, as: $J_o = J_{Bo} = 5.3080 \times 10^{-17}\ \left(\frac{A}{cm^2}\right)$, calculated for (r_S, r_{Tl}).

It should be noted that these values of J_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 J_{sc}, fill factor FF, and photovoltaic conversion efficiency η, 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]:

$$V_{oc1} = 624\ \text{mV},\ J_{sc1} = 36.3\ \frac{\text{mA}}{\text{cm}^2},\ FF_1 = 80.1\ \% \tag{48}$$

and the second one by [23, 28]:

$$V_{oc2} = 740\ \text{mV}, J_{sc2} = 41.8\ \frac{\text{mA}}{\text{cm}^2},\ FF_2 = 82.7\ \%. \tag{49}$$

In the following, we will develop our empirical treatment method of two points, used to determine J_{sc} and FF, basing on accurate results given in Equations (48) and (49).

6. Photovoltaic Conversion Effect

The well-known net current density J at T=300 K, expressed as a function of the applied voltage V, flowing through the $n^+ - p$ junction of silicon solar cells, is defined by:

$$J(V) \equiv J_{ph.}(V) - J_o \times \left(e^{\frac{V}{n(V) \times V_T}} - 1\right), V_T \equiv \frac{k_B T}{e} = 25.8543\ \text{mV} \tag{50}$$

Noting that $J(V) = 0$ at $V = V_{oc}$, V_{oc} being an open circuit voltage, at which $J_{ph.}(V = V_{oc}) \equiv J_{sc}(W,N,r_d,S,N_a,r_a,V_{oc})$, where J_{sc} is the short circuit current density. Here, $J_{ph.}$ is the photocurrent density and $J_o(W,N,r_d,S,N_a,r_a) \equiv J_{Eo} + J_{Bo}$ is the "dark saturation current density" or the $n^+ - p$ junction leakage saturation current density in the absence of light, defined in Equation (47). Therefore, the photovoltaic conversion effect occurs, according to:

$$J_{sc}(W,N,r_d,S,N_a,r_a,V_{oc}) \equiv J_o(W,N,r_d,S,N_a,r_a) \times (e^{v} - 1), v(W,N,r_d,S,N_a,r_a,V_{oc}) \equiv \frac{V_{oc}}{n \times V_T} \tag{51}$$

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

$$n(W,N,r_d,S,N_a,r_a,V_{oc}) = n_1(W,N,r_d,S,N_a,r_a,V_{oc1},J_{sc1}) + n_2(W,N,r_d,S,N_a,r_a,V_{oc2},J_{sc2}) \times \left(\frac{V_{oc}}{V_{oc1}} - 1\right)^{y_n}, \tag{52}$$

$$y_n = 1.1248$$

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

$$n_{1(2)}\left(W, N, r_d, S, N_a, r_a, V_{oc1(2)}, J_{sc1(2)}\right) \equiv \frac{V_{oc1(2)}}{V_T} \times \frac{1}{\ln\left(\frac{J_{sc1(2)}}{J_o} + 1\right)} \tag{53}$$

implying that both $n_{1(2)}$ (or n) and J_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:

$$W = 4.4 \text{ nm} = 0.0044 \text{ µm}, N = 10^{20} \text{ cm}^{-3}, r_d = r_P, S = 10^{50} \frac{\text{cm}}{\text{s}}, N_a = 10^{16} \text{ cm}^{-3}, r_a = r_B \tag{54}$$

the exponent $y_n = 1.1248$ was chosen such that:

$$n\left(W, N, r_d, S, N_a, r_a, V_{oc1(2)}\right) \equiv n_{1(2)}\left(W, N, r_d, S, N_a, r_a, V_{oc1(2)}, J_{sc1(2)}\right) = 1.2344\ (1.4534) \text{ respectively.}$$

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_o 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 $e^{v \equiv \frac{V_{oc}}{n \times V_T}}$.

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

$$FF_{1(2)}\left(W, N, r_d, S, N_a, r_a, V_{oc1(2)}\right) = \frac{v\left(W, N, r_d, S, N_a, r_a, V_{oc1(2)}\right) - \ln\left[v\left(W, N, r_d, S, N_a, r_a, V_{oc1(2)}\right) + 0.72\right]}{v\left(W, N, r_d, S, N_a, r_a, V_{oc1(2)}\right) + z_{FF_{1(2)}}} \tag{55}$$

where $z_{FF_{1(2)}} = 1.1\ (0.472)$ 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, $z_{FF_{1(2),\,Green}} = 1$, as proposed by Green [4].

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

$$\begin{aligned}\mathrm{FF}(\mathrm{W,N,r_d,S,\ N_a,r_a,V_{oc}}) \\ &= \mathrm{FF_1(W,N,r_d,S,\ N_a,r_a,V_{oc1}) + FF_2(W,N,r_d,S,\ N_a,r_a,V_{oc2})} \\ &\times \left(\frac{\mathrm{V_{oc}}}{\mathrm{V_{oc1}}} - 1\right)^{y_{FF}},\end{aligned} \quad (56)$$

$$y_{FF} = 2.0559$$

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

Then, the photovoltaic conversion efficiency η can be defined by:

$$\eta(\mathrm{W,N,r_d,S,\ N_a,r_a,V_{oc}}) \equiv \frac{\mathrm{J_{sc} \times V_{oc} \times FF}}{\mathrm{P_{in.}}} \quad (57)$$

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

In summary, all above parameters such as: n, $\mathrm{J_{sc}}$, FF and η, defined in above, strongly depend on $\mathrm{J_o}$, determined in Equation (47), which is thus a central result of the present paper.

Now, for given physical conditions such as: $\mathrm{W,N,r_d,S,\ N_a}$ and $\mathrm{r_a}$, and by taking into account all remarks given in Table 5 and also in above Equation (53), our numerical results of n, $\mathrm{J_{sc}}$, FF and η, expressed as functions $\mathrm{V_{oc}}$, are respectively computed by using Equations (52, 51, 56, 57), and reported in following Table 6 and Figures 7, 8 and 9.

In Table 6, in which, for $624 \leq \mathrm{V_{oc}(mV)} \leq 750$ [23, 24, 27-29] the physical conditions used are:

$$\mathrm{W} = 0.206\ \mathrm{nm},\mathrm{N} = 10^{20}\ \mathrm{cm^{-3}},\mathrm{r_d} \equiv \mathrm{r_P},\mathrm{S} = 10^{50}\frac{\mathrm{cm}}{\mathrm{s}},\ \mathrm{N_a} = 10^{16}\ \mathrm{cm^{-3}},\ \mathrm{r_a} \equiv \mathrm{r_B} \quad (58)$$

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

Table 6. With the physical conditions given in Equation (58), our present results (PR) of n, $\mathrm{J_{sc}}(\frac{\mathrm{mA}}{\mathrm{cm^2}})$, 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: RD=$|1-(\mathrm{PR}/\mathrm{Data})|$.

Data (D) from References	V_{oc} (mV)	n	$J_{sc(PR)}(J_{sc(D)})$;RD	$FF_{(PR)}(FF_{(D)})$;RD	$\eta_{(PR)}(\eta_{(D)})$;RD
[28]	750	1.7474	40.24 (39.5); 1.9	80.58 (83.2); 3.1	24.32 (24.7); 1.5
[23,28]	740	1.7222	41.01 (41.8); 1.9	80.11 (82.7); 3.1	24.31 (25.6); <u>5.0</u>
[28]	738	1.7172	41.16 (40.8); 0.9	80.02 (83.5); 4.2	24.31 (25.1); 3.2
[28]	737	1.7146	41.23 (41.3); 0.2	80.00 (82.7); 3.3	24.30 (25.2); 3.6
[28]	718	1.6676	42.43 (42.1); 0.8	79.22 (83.2); 4.8	24.13 (25.1); 3.8
[24]	710	1.6481	42.82 (42.3); 1.2	78.95 (82.6); 4.4	24.00 (24.8); 3.2
[28,29]	706	1.6384	42.98 (42.7); 0.6	78.82 (82.8); 4.8	23.91 (25.0); 4.3
[24]	705	1.6360	43.02 (42.2); 1.9	77.87 (83.1); 6.3	23.89 (24.7); 3.3
[24]	703	1.6312	43.08 (42.0); 2.6	78.73 (82.7); 4.8	23.84 (24.4); 2.3
[28]	695	1.6122	43.30 (40.2); 7.7	78.50 (80.5); 2.5	23.62 (22.5); 4.9
[28]	680	1.5772	43.37 (40.5); 7.1	78.14 (80.3); 2.7	23.05 (22.1); 4.3
[29]	671.7	1.5584	43.20 (40.5); 6.5	77.98 (80.9); 3.6	22.63 (22.0); 2.8
[28]	667	1.5479	43.01 (39.8); <u>8.1</u>	77.91 (80.0); 2.6	22.35 (21.3); 4.9
[27]	665	1.5434	43.91 (42.2); 1.7	76.87 (78.7); 1.0	22.22 (22.1); 0.5
[24]	655	1.5217	42.21 (39.8); 6.1	77.74 (79.4); 2.1	21.50 (20.7); 3.8
[28]	643	1.4968	40.83 (39.3); 3.9	77.64 (83.6); <u>7.1</u>	20.38 (21.1); 3.4
[27]	632	1.4758	38.80 (39.2); 1.0	77.59 (75.8); 2.4	19.02 (18.7); 1.7
[27]	624	1.4630	36.30 (36.3); 0.0	77.58 (80.1); 3.1	17.57 (18.1); 2.9

The underlined RD(%)-values are the maximal ones.

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

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

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:

- in the Figure 7 (a), the function n determined in Equation (52) (or the function J_o given in Table 5) decreases from the CTER to the COER
- in Figures 7 (b), 7 (c) and 7(d), the functions J_{sc}, FF and η therefore increase from the CTER to the COER, and
- in Figure 7 (d), for the physical functions: W=85 μm and $S = 10^{-50}$ cm/s, the function η reaches a maximum equal to 27.77% at V_{oc}=715 mV; here 1 μm $= 10^{-6}$ m.

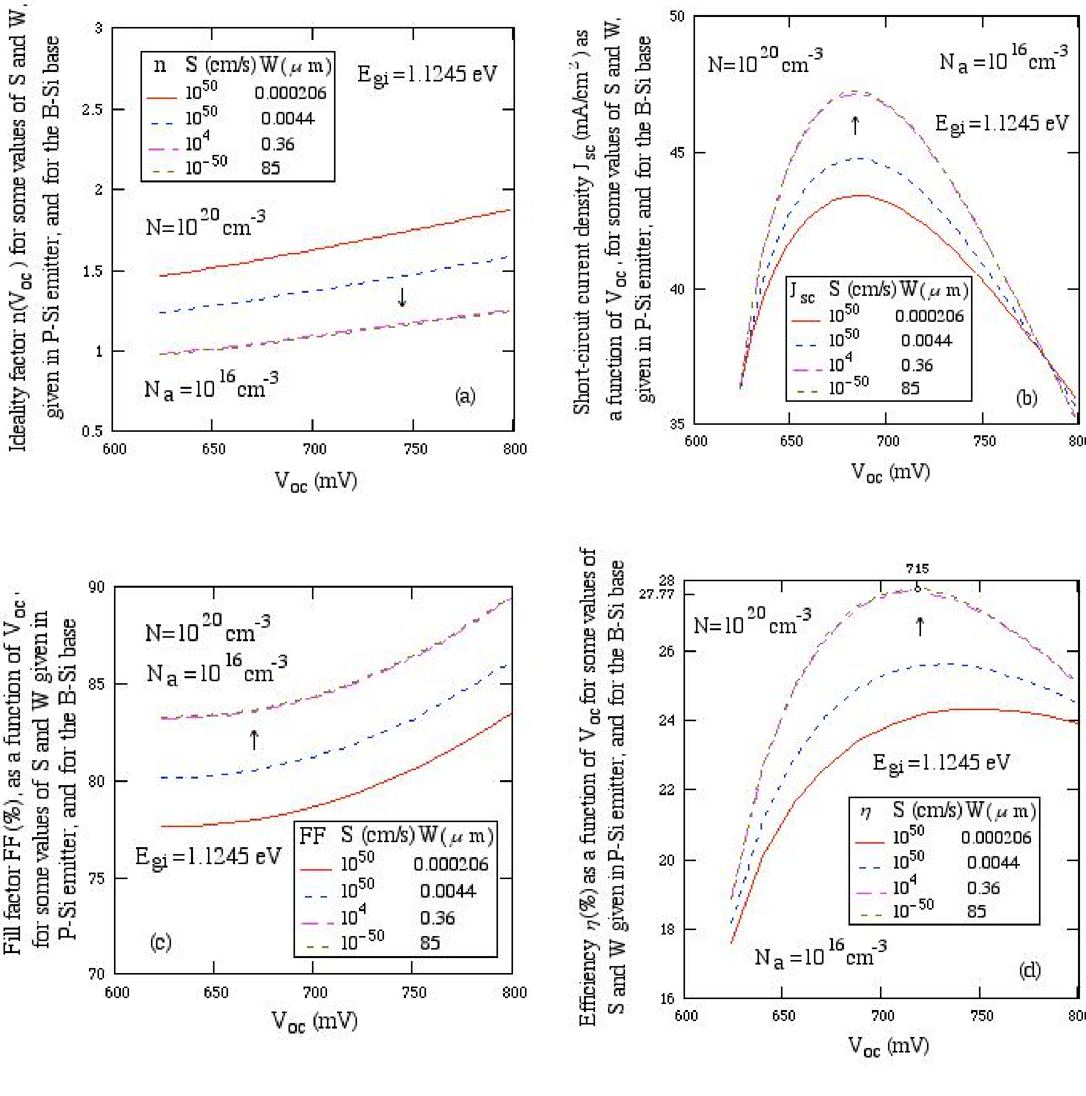


Figure 7. (a) Our n-results, (b) $J_{sc}(\frac{mA}{cm^2})$-results, (c) FF(%)-results, and (d) η(%)-results, plotted as functions of V_{oc} and obtained with increasing W and decreasing S (or from the completely transparent emitter region to the completely opaque emitter region).

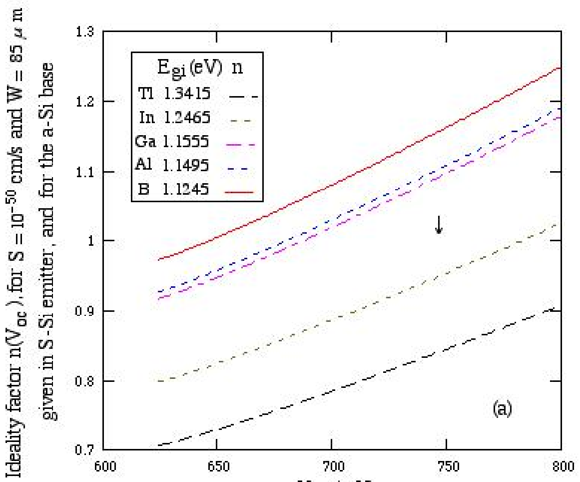
In Figures 8 (a), (b), (c) and (d), the physical conditions used are:

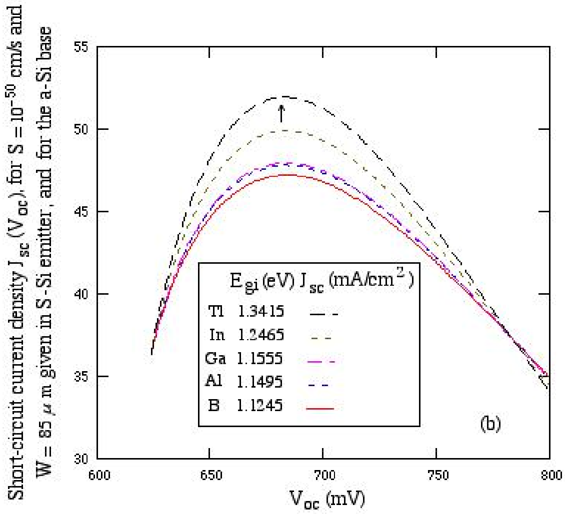
$$W = 85\ \mu m,\ N = 5 \times 10^{20}\ cm^{-3}, r_d = r_S,\ S = 10^{-50}\frac{cm}{s}, \tag{60}$$

$$N_a = 10^{16}\ \mathrm{cm}^{-3},\ r_a, \text{and } E_{gi}(r_a) \text{ at } 300\ \mathrm{K}$$

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

- in the Figure 8 (a), the function n determined in Equation (52) (or the function J_o given in Table 5) decreases (↓), and
- in Figures 8 (b), (c), (d), the functions J_{sc}, FF and η therefore increase (↑), and in particular, in Figure 8 (d), for the completely opaque (S-Si) emitter-region conditions, where J_{Eo}=0 or $J_o = J_{Bo}$, the maximal η-values are equal to: 27.77 %,…, 31.55 %, at V_{oc}=715 mV,…,703 mV, according to the E_{gi}-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.





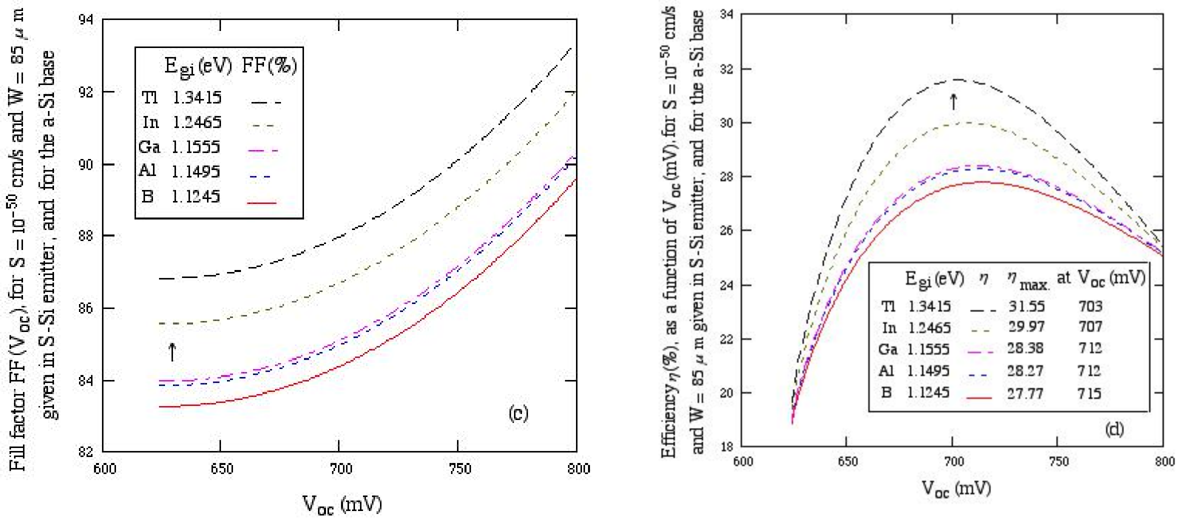


Figure 8. For $N = 5 \times 10^{20}\ cm^{-3}$ and $N_a = 10^{16}\ cm^{-3}$, (a) our n-results, (b) $J_{sc}(\frac{mA}{cm^2})$-results, (c) FF(%)-results, and (d) η(%)- results, plotted as functions of V_{oc} and obtained in the COER-conditions.

Finally, in Figures 9 (a), (b), (c) and (d), the physical conditions used are:

$$W = 0.000206\ \mu m,\ N = 5 \times 10^{20}\ cm^{-3},\ r_d,\ S = 10^{50}\frac{cm}{s},$$
$$N_a = 10^{16}\ cm^{-3},\ r_{Tl},\ \text{and}\ E_{gi}(r_d)\ \text{at 300 K} \tag{61}$$

according to the CTER, and they are also given in Table 5 for the third case. Here, the values of $E_{gi}(r_d)$ at 300 K are given in Table 2. Then, the numerical results of n, J_{sc}, FF and η are calculated, using Equations (52, 51, 56, 57). Further, for a given V_{oc} and with increasing r_a-values, it should be concluded that, due to the donor-size effect,

- in the Figure 9 (a), the function n determined in Equation (52) (or the function J_o given in Table 5) decreases (↓), and
- in Figures 9 (b), (c), (d), the functions J_{sc}, FF and η therefore increase (↑), and in particular, in Figure 9 (d), in the conditions of completely transparent and heavily doped (donor-Si) emitter-and- lightly doped (Tl-Si) base regions, the maximal η-values are equal to: 24.28 %,…, 31.51 %, at V_{oc}=748 mV,…,703 mV, according to the E_{gi}-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 8 (d).

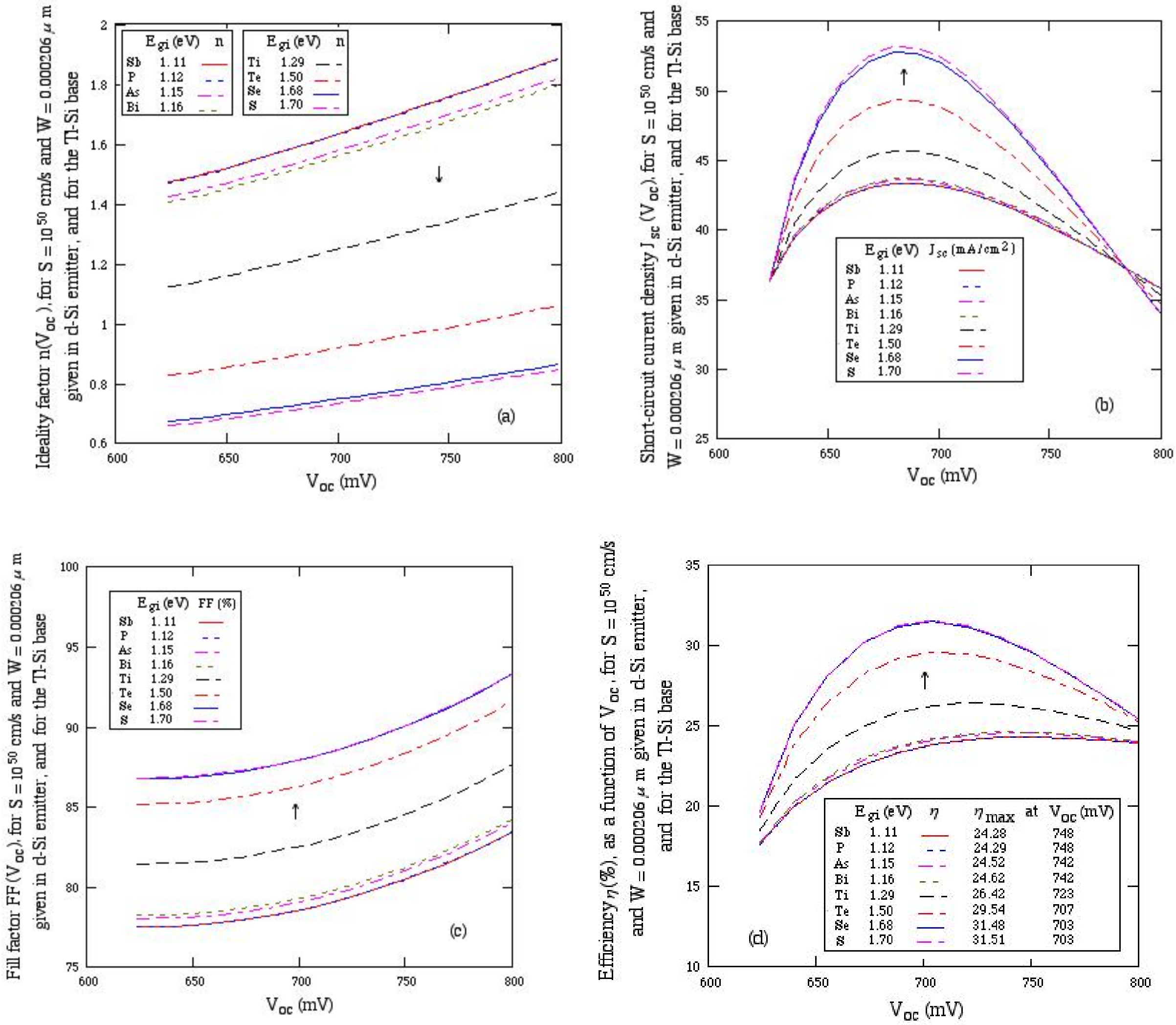


Figure 9. For $N = 5 \times 10^{20}$ cm^{-3} and $N_a = 10^{16}$ cm^{-3}, (a) our n-results, (b) $J_{sc}(\frac{mA}{cm^2})$-results, (c) FF(%)-results, and (d) η(%)- results, plotted as functions of V_{oc} and obtained in the CTER-conditions.

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: $J_o \equiv J_{Eo} + J_{Bo}$, as given in Sections 4, 5 and 6. Then, some concluding remarks are obtained and discussed as follows.

1. Using the optical band gap (E_{g1})-data given by Wagner and del Alamo [44], our E_{g1}-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_{Eo}-data, given by del Alamo et al. [10, 12], by using Equation (44), our J_{Eo}-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_{Eo}-results, obtained by those authors, are accurate within 36% [10, 12]. Our present accurate expression for J_{Eo} is thus imperative for continuing the performance improvement of solar cell systems.

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_o) have the same variations, which strongly affect other (V_{oc}, J_{sc}, FF, η)-results, as discussed in Eq. (53), indicating that J_o, 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, η)-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 η, suggesting thus a probable accuracy of J_{Bo} ($\leq 8.1\%$), since our J_{Eo}-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 8 (d), and 24.28%, …, 31.51%, as observed in Figure 9 (d), noting that our obtained highest η-values are found to be almost equal, as: 31.51%$\simeq$ 31.55%. This probably comes from the fact that in the limiting case of the physical conditions given Eq. (60), defined as: r_S and $r_a = r_{Tl}$, we obtain: $J_o = J_{Bo} = 5.3080 \times 10^{-17} \left(\frac{A}{cm^2}\right)$, as given in Table 5 for the second case, and in other limiting case of the physical conditions given Eq. (61), defined as: $r_d = r_S$ and r_{Tl}, we get: $J_o = 5.7767 \times 10^{-17} \left(\frac{A}{cm^2}\right) \simeq J_{Bo} = 5.3080 \times 10^{-17} \left(\frac{A}{cm^2}\right)$, as seen in Table 5 for the third case.

In summary, being due to the impurity-size effects, our limiting value of η_1=31.55%, as that given in Figure 8 (d), is thus obtained in the following limiting physical conditions as:

$$W = 85\ \mu m,\ N = 5 \times 10^{20}\ cm^{-3}, E_{gi}(r_d = r_S) = 1.7035\ eV,\ S = 10^{-50} \frac{cm}{s},$$

$$N_a = 10^{16}\ cm^{-3},\ \text{and}\ E_{gi}(r_a = r_{Tl}) = 1.3415,\ \text{at}\ 300\ K,$$

η_2 =27.77%, as that given in Figure 7 (d), is obtained in the following limiting physical conditions as:

$$\mathrm{W} = 85\ \mu\mathrm{m}, \mathrm{N} = 10^{20}\ \mathrm{cm}^{-3}, \mathrm{E_{gi}}(\mathrm{r_d} = \mathrm{r_P}) = 1.1245\ \mathrm{eV}, \mathrm{S} = 10^{-50}\frac{\mathrm{cm}}{\mathrm{s}},$$

$$\mathrm{N_a} = 10^{16}\ \mathrm{cm}^{-3},\ \text{and}\ \mathrm{E_{gi}}(\mathrm{r_a} = \mathrm{r_B}) = 1.1245, \text{at 300 K},$$

and η_3 =27.77%, as that given in Figure 8 (d), is thus obtained in the following limiting physical conditions as:

$$\mathrm{W} = 85\ \mu\mathrm{m}, \mathrm{N} = 5 \times 10^{20}\ \mathrm{cm}^{-3}, \mathrm{E_{gi}}(\mathrm{r_d} = \mathrm{r_S}) = 1.7035\ \mathrm{eV}, \mathrm{S} = 10^{-50}\frac{\mathrm{cm}}{\mathrm{s}},$$

$$\mathrm{N_a} = 10^{16}\ \mathrm{cm}^{-3},\ \text{and}\ \mathrm{E_{gi}}(\mathrm{r_a} = \mathrm{r_B}) = 1.1245\ \mathrm{eV}, \text{at 300 K}.$$

Those limiting $\eta_{1,2,3}$–results can be compared with that obtained by Richter et al. (R) [26], η_R =29.43%, for a thick $100\ \mu\mathrm{m}$ solar cell made of un-doped silicon, as: $\eta_2 = \eta_3 < \eta_R < \eta_1$, being probably due to the impurity-size effects.

Finally, it should be noted that the effects of heavy doping and impurity size on minority-carrier transport parameters in heavily (lightly) doped p(n)-type crystalline silicon at 300 K, applied to determine the performance of $\mathrm{p^+ - n}$ junction solar cells, could be investigated by a similar empirical treatment method.

Acknowledgments: We thank Prof. Dr. Nghi Q. Lam, the Former Editor-in-Chief of Applied Physics Letters (1994-2014), for his helpful remarks and suggestions, which have greatly improved the presentation of our paper.

Appendices

Appendix A: Fermi Energy

0The Fermi energy $\mathrm{E_F}$, obtained for any T and donor density N, being investigated in our previous paper, with a precision of the order of 2.11×10^{-4} [39], is now summarized in the following. First of all, we define the reduced electron density by:

$$\mathrm{u}(\mathrm{N},\mathrm{T},\mathrm{r_d},\mathrm{g_c}) \equiv \frac{\mathrm{N}}{\mathrm{N_c}(\mathrm{T},\mathrm{r_d},\mathrm{g_c})} \equiv \mathcal{F}_{1/2}(\theta) \quad \text{(A1)}$$

where $\mathrm{N_c}$ is defined in Eq. (6), $\theta(\mathrm{u}) \equiv \frac{\mathrm{E_F(u)}}{\mathrm{k_B T}}$ is the reduced Fermi energy, and $\mathcal{F}_{1/2}(\theta)$ is the Fermi-Dirac integral, defined by [40]:

$$\mathcal{F}_{\frac{1}{2}}(\theta) \equiv \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{x^{\frac{1}{2}} dx}{1 + e^{x-\theta}}, x \equiv \frac{E}{k_B T} \tag{A2}$$

which was calculated for any values of θ, 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 $u \equiv \mathcal{F}_{1/2}(\theta)$ 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]:

$$\theta(u) \equiv \frac{E_F(u)}{k_B T} = \frac{G(u) + Au^B F(u)}{1 + Au^B}, \text{with } A = 0.0005372 \text{ and } B = 4.82842262 \tag{A3}$$

where, in the degenerate case or when $\theta(u \gg 1) \to \infty$, Equation (A3) is reduced to:

$F(u) = au^{\frac{2}{3}}\left(1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}}\right)^{-\frac{2}{3}}$; $a = [3\sqrt{\pi}/4]^{2/3}$, $b = \frac{1}{8}\left(\frac{\pi}{a}\right)^2$, and $c = \frac{62.3739855}{1920}\left(\frac{\pi}{a}\right)^4$,

and in the non-degenerate case or when $\theta(u \ll 1) \ll 0$, to:

$$G(u) \simeq \mathrm{Ln}(u) + 2^{-\frac{3}{2}} \times u \times e^{-du}, d = 2^{3/2}\left[\frac{1}{\sqrt{27}} - \frac{3}{16}\right] > 0$$

Appendix B: Approximate Form for Band Gap Narrowing (BGN)

First of all, we will normalize the various energies by using the effective Rydberg energy R, as:

$$R(T,r_d) = 13.605693 \times \frac{m_c(T,r_d)}{\varepsilon^2(r_d)} (eV) \tag{A4}$$

and we express the effective Wigner-Seitz radius r_s characteristic of the interactions by:

$$r_s(N,T,r_d,g_c) \equiv \left(\frac{3g_c}{4\pi N}\right)^{\frac{1}{3}} \times \frac{1}{a_B(T,r_d)}$$

Here, $a_B(T,r_d) = 5.2917715 \times 10^{-9} \times \frac{\varepsilon(r_d)}{m_c(T,r_d)}$ (cm) is the Bohr radius. Therefore, one has:

$$r_s(N,T,r_d,g_c) = 1.1723 \times 10^8 \times \left(\frac{g_c}{N}\right)^{1/3} \times \frac{m_c(T,r_d)}{\varepsilon(r_d)} \tag{A5}$$

Therefore, the ratio R/r_s is thus proportional to: $\frac{\varepsilon(r_P)}{\varepsilon(r_d)} \times N_r^{1/3}$, where $N_r \equiv \left(\frac{6 \times N}{g_c \times 9.999 \times 10^{17}\ cm^{-3}}\right)$. Now, an empirical expression for BGN is proposed by:

$$\Delta E_g(N,T,r_d,g_c) = \Delta E_{g(XE)} + \Delta E_{g(e-cor)} + \Delta E_{g(h-cor)} + \Delta E_{g(e-D)} + \Delta E_{g(h-D)} + \Delta E_{g(LT)} \equiv - R \times \mu_{XE}(r_s) - R\times \mu_c(r_s) - R \times \mu_n^{h-Cor}(r_s) - R \times \mu_n^{e-D}(r_s) - R \times \mu_n^{h-D}(r_s) + \Delta E_{g(LT)} \quad (A6)$$

where, R and r_s are defined above, and five first contributions of the spin-polarized chemical potential energy μ were determined in our previous paper [42], and sixth μ-one by Lanyon and Tuft [6]. Further, the BGN-results such as: $\Delta E_{g(XE)}$, $\Delta E_{g(e-cor)}$, $\Delta E_{g(h-cor)}$, $\Delta E_{g(e-D)}$, $\Delta E_{g(h-D)}$, and $\Delta E_{g(LT)}$ will be respectively determined in the following.

(i) The first $\left[\Delta E_{g(XE)} \equiv - R \times \mu_{XE}(r_s)\right]$-term of Equation (A6) represents the shift in majority conduction-band edge, due to the exchange energy (XE) of an effective electron gas, being proportional to: R/r_s or to: $\frac{\varepsilon(r_P)}{\varepsilon(r_d)} \times N_r^{1/3}$. Therefore, one has:

$$\Delta E_{g(XE)} \simeq a_1 \times \frac{\varepsilon(r_P)}{\varepsilon(r_d)} \times N_r^{1/3} \quad (A7)$$

where the constant a_1 was chosen to be equal to 3.8×10^{-3} (eV).

(ii) The second $\left[\Delta E_{g(e-cor)} \equiv - R\times \mu_c(r_s)\right]$-term of Equation (A6) represents the shift in majority conduction-band edge, due to the correlation energy of an effective electron gas, $E_c(r_s)$, and given by [42]:

$$E_c(N,T,r_d,g_c) = \frac{-0.87553}{0.0908 + r_s} + \frac{\frac{0.87553}{0.0908 + r_s} + \left(\frac{2[1-\ln(2)]}{\pi^2}\right) \times \ln(r_s) - 0.093288}{1 + 0.03847728 \times r_s^{1.67378876}} \quad (A8)$$

noting that from the a Seitz's theorem [42], one has:

$$\mu_c(N,T,r_d,g_c) \equiv \frac{-r_s^4}{3} \times \frac{\partial}{\partial r_s} \frac{E_c(r_s)}{r_s^3} = - E_c(r_s) + \frac{r_s}{3} \times \frac{\partial}{\partial r_s} E_c(r_s) \simeq 2.503 \times [-E_c(r_s)] \equiv \mu_{c(A)}(r_s) \quad (A9)$$

Moreover, our numerical calculation indicates that the approximate form for $\mu_c(r_s)$, $\mu_{c(A)}(r_s)$, is accurate within 1.87% for $g_c = 6$ in various donor-Si systems, noting that the relative error of $\mu_{c(A)}(r_s)$ is defined as: $1 - \frac{\mu_{c(A)}(r_s)}{\mu_c(r_s)}$. Therefore, from Equations (A4, A5, A8, A9), an approximate form for $\Delta E_{g(e-cor)} \equiv - R\times \mu_c(r_s) \simeq 2.503 \times [-R \times E_c(r_s)]$, being proportional to: $\left(\frac{R}{r_s}\right) \times (2.503 \times [-E_c(r_s) \times r_s])$, is found to be given by:

$$\Delta E_{g(e-cor)} \simeq a_2 \times \frac{\varepsilon(r_P)}{\varepsilon(r_d)} \times N_r^{\frac{1}{3}} \times (2.503 \times [-E_c(r_s) \times r_s]) \tag{A10}$$

where the constant a_2 was chosen to be equal to 6.5×10^{-4} (eV).

(iii) The third $[\Delta E_{g(h-cor)} \equiv -R \times \mu_n^{h-Cor}(r_s)]$-term of Equation (A6) is the spin-polarized ground-state energy at the wave number k=0, due to the minority hole-correlation or screened Coulomb hole-correlation, being obtained by the plasmon-pole approximation and thus proportional to: $\frac{R}{r_s^{3/4}} \times \sqrt{\frac{m_v(T)}{m_c(T,r_d)}}$ [42]. That thus gives:

$$\Delta E_{g(h-cor)} \simeq a_3 \times \left[\frac{\varepsilon(r_P)}{\varepsilon(r_d)}\right]^{5/4} \times \left[\frac{m_c(T,r_d)}{m_c(T,r_P)}\right]^{1/4} \times N_r^{1/4} \times \sqrt{\frac{m_v(T)}{m_c(T,r_d)}} \tag{A11}$$

where the constant a_3 was chosen to be equal to 2.8×10^{-3} (eV).

(iv) The fourth $[\Delta E_{g(e-D)} \equiv -R \times \mu_n^{e-D}(r_s)]$-term of Equation (A6) is the spin-polarized chemical potential energy, due to the majority electron-donor (e-D) interaction screened Coulomb potential energy, being obtained by a second-order perturbation approximation and proportional to: $\frac{R}{r_s^{3/2}}$ [42]. Therefore, one has:

$$\Delta E_{g(e-D)} \simeq a_4 \times \sqrt{\frac{m_c(T,r_P) \times \varepsilon(r_P)}{m_c(T,r_d) \times \varepsilon(r_d)}} \times N_r^{1/2} \tag{A12}$$

where the constant a_4 was chosen to be equal to 5.597×10^{-3} (eV).

(v) The fifth $[\Delta E_{g(h-D)} \equiv -R \times \mu_n^{e-D}(r_s)]$-term of Equation (A6) is the spin-polarized chemical potential energy, due to the minority hole-D interaction screened Coulomb potential energy, being also obtained by a second-order perturbation approximation and now proportional to: $\sqrt{\frac{m_v(T) \times \varepsilon(r_P)}{m_v(T) \times \varepsilon(r_d)}} \times N_r^{1/2}$ [42]. Here, one has:

$$\Delta E_{g(h-D)} \simeq a_5 \times \sqrt{\frac{\varepsilon(r_P)}{\varepsilon(r_d)}} \times N_r^{1/2} \tag{A13}$$

where $a_5 \equiv a_4$.

(vi) Finally, the sixth $\Delta E_{g(LT)}$-term of Equation (A6) is the BGN, which was determined by Lanyon [6], basing on the basic concept that the charge of minority hole attracts to its majority electrons of the opposite polarity, producing a screened Coulomb potential, with a screening length L_s, being proportional to: $N^{-1/6} \times \sqrt{\frac{\varepsilon(r_d)}{m_c(T,r_d)}}$ [6]. Further, because of the electrostatic force between the charges, the work must be done to separate them since the paired charges have a lower energy than when each is isolated. This reduction in energy or the BGN can be shown to be proportional to: $\frac{1}{\varepsilon(r_d) \times L_s}$, [6] or to: $\left[\frac{m_c(T,r_d)}{m_c(T,r_P)}\right]^{1/2} \times \left[\frac{\varepsilon(r_P)}{\varepsilon(r_d)}\right]^{\frac{3}{2}} \times N_r^{\frac{1}{6}}$. Therefore, one has:

$$\Delta E_{g(LT)} \simeq a_6 \times \left[\frac{m_c(T,r_d)}{m_c(T,r_P)}\right]^{1/2} \times \left[\frac{\varepsilon(r_P)}{\varepsilon(r_d)}\right]^{\frac{3}{2}} \times N_r^{\frac{1}{6}} \tag{A14}$$

where the constant a_6 was chosen to be equal to 8.1×10^{-4} (eV).

In summary, replacing Equations (A7, A10-A14) into Equation (A6), we thus obtain an approximate expression for the BGN as:

$$\begin{aligned}\Delta E_g(N,T,r_d,g_c) \simeq\ & a_1 \times \frac{\varepsilon(r_P)}{\varepsilon(r_d)} \times N_r^{1/3} + a_2 \times \frac{\varepsilon(r_P)}{\varepsilon(r_d)} \times N_r^{\frac{1}{3}} \times (2.503 \times [-E_c(r_s) \times r_s]) \\ & + a_3 \times \left[\frac{\varepsilon(r_P)}{\varepsilon(r_d)}\right]^{5/4} \times \left[\frac{m_c(T,r_d)}{m_c(T,r_P)}\right]^{1/4} \times N_r^{1/4} \times \sqrt{\frac{m_v(T)}{m_c(T,r_d)}} + a_4 \\ & \times \sqrt{\frac{m_c(T,r_P) \times \varepsilon(r_P)}{m_c(T,r_d) \times \varepsilon(r_d)}} \times N_r^{1/2} \times \left\{1 + \sqrt{\frac{m_c(T,r_d)}{m_c(T,r_P)}}\right\} \\ & + a_6 \times \left[\frac{m_c(T,r_d)}{m_c(T,r_P)}\right]^{1/2} \times \left[\frac{\varepsilon(r_P)}{\varepsilon(r_d)}\right]^{\frac{3}{2}} \times N_r^{\frac{1}{6}}\end{aligned} \tag{A15}$$

noting that in the P-Si system at 300 K the above constants a_n, with n=1, 2, …, 6, were chosen such that for $g_c = 6$ the numerical results of minority-carrier saturation current J_{Eo} are found to be accurate within 1.78%, as seen in Table 4.

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