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Maximal Efficiencies in New Single $Si_{1-x}Ge_x$-Alloy Junction Solar Cells at 300 K

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Abstract:

In single $n^+(p^+) - p(n)$ $[X(x) \equiv Si_{1-x}Ge_x]$-alloy junction solar cells at 300 K, $0 \le x \le 1$, by basing on the same physical model and the same treatment method, as those used in our recent work (Van Cong et al., 2023; Van Cong, 2023), we will investigate the highest (or maximal) efficiencies, $\eta_{Imax.(IImax.)}$, obtained at the open circuit voltage $V_{oc}(= V_{ocI(ocII)})$, according to highest hot reservoir temperatures $T_H(K)$, obtained from the Carnot efficiency theorem, being proved by entropy law, in the following. **(i)**-First, in the single $n^+ - p$ $Si_{1-x}Ge_x$-alloy junction solar cell, from Table 3, with increasing x=(0, 0.5, 1) and for given $r_{Sn(Cd)}$-radius, for example, one obtains: $\eta_{Imax.}$(↘)= **28.21%**, 25.97%, **23.36%**, according to $T_H(K) = \mathbf{417.9}, 405.2, \mathbf{391.4}$, at $V_{ocI}(V) = \mathbf{0.70}, 0.71, \mathbf{0.74}$, noting that the values, marked in bold, correspond to those obtained respectively for x=(0, 1). **(ii)**- Secondly, in the single $p^+ - n$ $Si_{1-x}Ge_x$-alloy junction solar cell, from Table 5, with increasing x=(0, 0.5, 1) and for given $r_{Cd(Sn)}$-radius, for example, one obtains: $\eta_{IImax.}$(↘)= **27.66%**, 25.89%, **23.63%**, according to $T_H(K) = \mathbf{414.7}, 404.8, \mathbf{392.8}$, at $V_{ocI}(V) = \mathbf{0.71}, 0.72, \mathbf{0.76}$, noting that the values, marked in bold, correspond to those obtained respectively for x=(0, 1). **(iii)**- Then, as noted in (i) and (ii), for x=0, $\eta_{I(II)max.} = 28.21\ \%\ (27.66\ \%)$, which can be compared with the corresponding ones, 27.19 % and 26.7 %, obtained, for the single-junction Si crystalline solar cell, by Singh and Ravindra (2012) and by Green et al. (2022), respectively. **(iv)**- Further, as noted in (i) and (ii), for x=1, $\eta_{I(II)max.} = 23.36\%\ (23.63\%)$, which can be compared with the corresponding ones, 12.50 % and 14.82 %, obtained, for the single-junction Ge crystalline solar cell, by Singh and Ravindra (2012) and by Van Cong (2023), respectively. Finally, as discussed in above remarks (iii) and (iv), in order to obtain the highest efficiencies, the present single $Si_{1-x}Ge_x$-alloy junction solar cells could be chosen rather than the single crystalline (Si, Ge)-junction solar cells.

Keywords: *Single $Si_{1-x}Ge_x$-alloy junction solar cell, photovoltaic conversion factor, photovoltaic conversion effect.*

Introduction

In single $n^+(p^+) - p(n)$ $[X(x) \equiv Si_{1-x}Ge_x]$-alloy junction solar cells at 300 K, $0 \le x \le 1$, by basing on the same physical model and treatment method, as used in our recent work (Van Cong, 2023; Van Cong et al., 2023), and also other works (Green, 2022; Singh & Ravindra, 2012; Van Cong & Debiais, 1997, 1993; Van Cong et al., 1984), we will investigate the highest (or maximal) efficiencies, $\eta_{Imax.(IImax.)}$,

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according to highest hot reservoir temperatures $T_H(K)$, obtained at the open circuit voltage: $V_{oc} = V_{ocI(ocII)}$ and from the Carnot- efficiency theorem, being proved by entropy law.

In the following, we will show that the energy-band-structure parameters, due to the effects of x-Ge concentration, size impurity, temperature T and heavy doping, affect strongly the dark (or total) minority-carrier saturation current density and the photovoltaic conversion effect. Finally, some numerical results and concluding remarks will be presented and discussed.

Energy-Band-Structure Parameters and Dark Minority-Carrier Saturation Current Density, Due to the Effects of x- Ge Concentration, Impurity Size, and Heavy Doping

A. Effect of x-Ge concentration

In the $n^+(p^+) - p(n)$ single $n^+(p^+) - p(n)$ [X(x)≡ $Si_{1-x}Ge_x$]-alloy junction at T=0 K, the values of the intrinsic energy-band-structure parameters, such as: the effective average number of equivalent conduction (valence)-band edges $g_{c(v)}(x)$, the unperturbed relative effective electron (hole) mass in conduction (valence) bands $m_{c(v)}(x)/m_o$, m_o being the electron rest mass, the unperturbed relative dielectric constant $\varepsilon_o(x)$, the effective donor (acceptor)-ionization energy $E_{do(ao)}(x)$, and the isothermal bulk modulus $B_{do(ao)}(x) \equiv \frac{E_{do(ao)}(x)}{(4\pi/3)\times(r_{do(ao)})^3}$, at $r_{d(a)} = r_{do(ao)}$, noting that $r_{do(ao)} \equiv r_{Si} = 0.117$ nm for the $Si_{1-x}Ge_x$-alloy, are given respectively in the following,

$$g_c(x) = 4 \times x + 6 \times (1 - x), g_v(x) = 2 \times x + 2 \times (1 - x), \quad (1)$$

$$m_c(x)/m_o = 0.12 \times x + 0.3216 \times (1 - x), m_v(x)/m_o = 0.3 \times x + 0.3664 \times (1 - x), \quad (2)$$

$$\varepsilon_o(x) = 15.8 \times x + 11.4 \times (1 - x), \quad (3)$$

$$E_{go}(x) \text{ in eV} = 0.7412 \times x + 1.17 \times (1 - x), \quad (4)$$

$$E_{do(ao)}(x) = \frac{13600\times[m_{c(v)}(x)/m_o]}{[\varepsilon_o(x)]^2} \text{ meV, and} \quad (5)$$

$$B_{do(ao)}(x) \equiv \frac{E_{do(ao)}(x)}{(4\pi/3)\times(r_{do(ao)})^3}. \quad (6)$$

B. Effects of Impurity-size, with a given x

Here, one shows that the effects of $r_{d(a)}$ and x-Ge concentration strongly affect the changes in all the energy-band-structure parameters, being expressed in terms of the effective relative dielectric constant $\varepsilon(r_{d(a)}, x)$, are investigated as follows.

At $r_{d(a)} = r_{do(ao)}$, the needed boundary conditions are found to be, for the impurity-atom volume V= $(4\pi/3) \times (r_{d(a)})^3$, $V_{do(ao)} = (4\pi/3) \times (r_{do(ao)})^3$, for the pressure p, as: $p_o = 0$, and for the deformation potential energy (or the strain energy) σ, as: $\sigma_o = 0$. Further, the two important equations (Van Cong et al., 1984), used to determine the σ-variation: $\Delta\sigma \equiv \sigma - \sigma_o = \sigma$, are defined by: $\frac{dp}{dV} = -\frac{B}{V}$ and $p = -\frac{d\sigma}{dV}$. giving: $\frac{d}{dV}(\frac{d\sigma}{dV}) = \frac{B}{V}$. Then, by an integration, one gets:

$[\Delta\sigma(r_{d(a)},x)]_{n(p)} = B_{do(ao)}(x) \times (V - V_{do(ao)}) \times \ln\left(\frac{V}{V_{do(ao)}}\right) = E_{do(ao)}(x) \times \left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 \geq 0.$ (7a)

Furthermore, we also shown that, as $r_{d(a)} > r_{do(ao)}$ ($r_{d(a)} < r_{do(ao)}$), the compression (dilatation) gives rise to: the increase (the decrease) in the energy gap $E_{gn(gp)}(r_{d(a)},x)$, and in the effective donor (acceptor)-ionization energy $E_{d(a)}(r_{d(a)},x)$ in absolute values, being obtained from the effective Bohr model, and then such the compression (dilatation) is represented respectively by: $\pm [\Delta\sigma(r_{d(a)},x)]_{n(p)}$,

$$E_{gn(gp)}(r_{d(a)},x) - E_{go}(x) = E_{d(a)}(r_{d(a)},x) - E_{do(ao)}(x) = E_{do(ao)}(x) \times \left[\left(\frac{\varepsilon_o(x)}{\varepsilon(r_{d(a)})}\right)^2 - 1\right] = + [\Delta\sigma(r_{d(a)},x)]_{n(p)},$$

for $r_{d(a)} \geq r_{do(ao)}$, and for $r_{d(a)} \leq r_{do(ao)}$,

$$E_{gn(gp)}(r_{d(a)},x) - E_{go}(x) = E_{d(a)}(r_{d(a)},x) - E_{do(ao)}(x) = E_{do(ao)}(x) \times \left[\left(\frac{\varepsilon_o(x)}{\varepsilon(r_{d(a)})}\right)^2 - 1\right] = - [\Delta\sigma(r_{d(a)},x)]_{n(p)}. \quad (7b)$$

Therefore, from above Equations 7a and 7b, one obtains the expressions for relative dielectric constant $\varepsilon(r_{d(a)},x)$ and energy band gap $E_{gn(gp)}(r_{d(a)},x)$, as:

(i)-for $r_{d(a)} \geq r_{do(ao)}$, since $\varepsilon(r_{d(a)},x) = \frac{\varepsilon_o(x)}{\sqrt{1 + \left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3}} \leq \varepsilon_o(x)$,

$$E_{gn(gp)}(r_{d(a)},x) - E_{go}(x) = E_{d(a)}(r_{d(a)},x) - E_{do(ao)}(x) = E_{do(ao)}(x) \times \left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 \geq 0, \quad (8a)$$

according to the increase in both $E_{gn(gp)}(r_{d(a)},x)$ and $E_{d(a)}(r_{d(a)},x)$, for a given x, and

(ii)-for $r_{d(a)} \leq r_{do(ao)}$, since $\varepsilon(r_{d(a)},x) = \frac{\varepsilon_o(x)}{\sqrt{1 - \left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3}} \geq \varepsilon_o(x)$, with a condition, given by: $\left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 < 1$,

$$E_{gn(gp)}(r_{d(a)},x) - E_{go}(x) = E_{d(a)}(r_{d(a)},x) - E_{do(ao)}(x) = -E_{do(ao)}(x) \times \left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 \leq 0, \quad (8.b)$$

corresponding to the decrease in both $E_{gn(gp)}(r_{d(a)}, x)$ and $E_{d(a)}(r_{d(a)}, x)$, for a given x.

C. Effect of temperature T, with given x and $r_{d(a)}$

Here, the intrinsic band gap $E_{gin(gip)}(r_{d(a)}, x, T)$ at any T is given by (Van Cong, 2023; Van Cong et al., 2023):

$$E_{gin(gip)}(r_{d(a)}, x, T) \text{ in eV} = E_{gn(gp)}(r_{d(a)}, x) - 10^{-4} \times T^2 \times \left[\frac{3.525 \times x}{T+94\text{ K}} + \frac{2.54 \times (1-x)}{T+204\text{ K}}\right], \quad (9)$$

which gives: $E_{gin(gip)}(r_{do(ao)}, x = 0, T = 0K) = 1.17$ eV and $E_{gin(gip)}(r_{do(ao)}, x = 1, T = 0K) = 0.7412$ eV $\simeq 0.74$ eV, and $E_{gin(gip)}(r_{do(ao)}, x = 0, T = 300$ K$) = 1.1246$ eV $\simeq 1.12$ eV and $E_{gin(gip)}(r_{do(ao)}, x = 1, T = 300$ K$) = 0.6607$ eV$\simeq 0.66$ eV, as seen in Table 1, suggesting also that, for given x and $r_{d(a)}$, $E_{gin(gip)}$ decreases with an increasing T.

Furthermore, in the n(p)-type X(x)-alloy, one can define the intrinsic carrier concentration $n_{in(ip)}$ by:

$$n^2_{i\,n(p)}(T, r_{d(a)}, x) \equiv N_c(T, x) \times N_v(T, x) \times \exp\left(\frac{-E_{gin(p)}(T, r_{d(a)}, x)}{k_B T}\right), \quad (10)$$

where $N_{c(v)}(T, x)$ is the conduction (valence)-band density of states, being defined as:

$$N_{c(v)}(T, x) = 2 \times g_{c(v)}(x) \times \left(\frac{m_{c(v)}(x) \times k_B T}{2\pi\hbar^2}\right)^{\frac{3}{2}} \ (\text{cm}^{-3}). \quad (11)$$

So, the numerical results of those parameters: $B_{do(ao)}(x)$, $\varepsilon(r_{d(a)}, x)$, $E_{d(a)}(r_{d(a)}, x)$, and $E_{gin(gip)}(r_{d(a)}, x, T)$, being calculated with the use of Equations 4, 5, 8a (8b) and 9, are reported in following Table 1 (Appendix 1).

D. Heavy Doping Effect, with given T, x and $r_{d(a)}$

Here, as given in our previous works (Van Cong, 2023; Van Cong & Debiais, 1993), the Fermi energy $E_{Fn}(-E_{Fp})$, band gap narrowing (BGN), and apparent band gap narrowing (ABGN), are reported in the following.

First, the Fermi energy $E_{Fn}(-E_{Fp})$, obtained for any T and any d(a)-density, $N_{d(a)}$, being investigated in our previous paper (Van Cong & Debiais, 1993), with a precision of the order of 2.11×10^{-4}, is found to be given by:

$$\frac{E_{Fn}(u)}{k_B T}\left(\frac{-E_{Fp}(u)}{k_B T}\right) = \frac{G(u) + Au^B F(u)}{1 + Au^B}, \ A = 0.0005372 \text{ and } B = 4.82842262, \quad (12)$$

where u is the reduced electron density, $u(N_{d(a)}, T, x) \equiv \frac{N_{d(a)}}{N_{c(v)}(T,x)}$, $F(u) = au^{\frac{2}{3}}\left(1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}}\right)^{-\frac{2}{3}}$, $a = \left[(3\sqrt{\pi}/4) \times u\right]^{2/3}$, $b = \frac{1}{8}\left(\frac{\pi}{a}\right)^2$, $c = \frac{62.3739855}{1920}\left(\frac{\pi}{a}\right)^4$, and $G(u) \simeq Ln(u) + 2^{-\frac{3}{2}} \times u \times e^{-du}$; $d = 2^{3/2}\left[\frac{1}{\sqrt{27}} - \frac{3}{16}\right] > 0$.

Here, one notes that: (i) as $u \gg 1$, according to the heavily doped (HD) [d(a)- $X(x)$- alloy] emitter region (ER)-case, or to the degenerate case, Eq. (12) is reduced to the function F(u), and (ii) $\frac{E_{Fn}(u \ll 1)}{k_B T}\left(\frac{-E_{Fp}(u \ll 1)}{k_B T}\right) \ll -1$, to the lightly doped (LD) [a(d)- $X(x)$ alloy] base region (BR)-case, or to the non-degenerate case, Eq. (12) is reduced to the function G(u).

Secondly, if denoting the effective Wigner-Seitz radius $r_{sn(sp)}$, characteristic of the interactions, by:

$$r_{sn(sp)}(N_{d(a)}, r_{d(a)}, x) = 1.1723 \times 10^8 \times \left(\frac{g_{c(v)}}{N_{d(a)}}\right)^{1/3} \times \frac{m_{c(v)}(x)}{\varepsilon(r_{d(a)}, x)}, \quad (13)$$

the correlation energy of an effective electron gas, $E_{cn(cp)}(N_{d(a)}, r_{d(a)}, x)$, is given as (Van Cong, 2023):

$$E_{cn(cp)}(N_{d(a)}, r_{d(a)}, x) = \frac{-0.87553}{0.0908 + r_{sn(sp)}} + \frac{\frac{0.87553}{0.0908 + r_{sn(sp)}} + \left(\frac{2[1 - ln(2)]}{\pi^2}\right) \times ln\,(r_{sn(sp)}) - 0.093288}{1 + 0.03847728 \times r_{sn(sp)}^{1.67378876}}.$$

Now, taking into account various spin-polarized chemical potential-energy contributions such as (Van Cong, 2023): exchange energy of an effective electron (hole) gas, majority-carrier correlation energy of an effective electron (hole) gas, minority hole (electron) correlation energy, majority electron (hole)-ionized d(a) interaction screened Coulomb potential energy, and finally minority hole (electron)-ionized d(a) interaction screened Coulomb potential energy, the band gap narrowing (BGN) are given as follows.

Then, in the n-type HD $X(x)$- alloy, the BGN is found to be given by (Van Cong, 2023):

$$\Delta E_{gn}(N_d, r_d, x) \simeq a_1 \times \frac{\varepsilon_o(x)}{\varepsilon(r_d, x)} \times N_r^{1/3} + a_2 \times \frac{\varepsilon_o(x)}{\varepsilon(r_d, x)} \times N_r^{\frac{1}{3}} \times (2.503 \times [-E_{cn}(r_{sn}) \times r_{sn}]) + a_3 \times \left[\frac{\varepsilon_o(x)}{\varepsilon(r_d, x)}\right]^{5/4} \times \sqrt{\frac{m_v}{m_c}} \times N_r^{1/4} + a_4 \times \sqrt{\frac{\varepsilon_o(x)}{\varepsilon(r_d, x)}} \times N_r^{1/2} \times 2 + a_5 \times \left[\frac{\varepsilon_o(x)}{\varepsilon(r_d, x)}\right]^{\frac{3}{2}} \times N_r^{\frac{1}{6}}, \quad N_r \equiv \left(\frac{N_d}{9.999 \times 10^{17}\ cm^{-3}}\right), \quad (14n)$$

where $a_1 = 3.8 \times 10^{-3}(eV)$, $a_2 = 6.5 \times 10^{-4}(eV)$, $a_3 = 2.8 \times 10^{-3}(eV)$, $a_4 = 5.597 \times 10^{-3}(eV)$ and $a_5 = 8.1 \times 10^{-4}(eV)$, and in the p-type HD $X(x)$- alloy, as:

$$\Delta E_{gp}(N_a, r_a, x) \simeq a_1 \times \frac{\varepsilon_o(x)}{\varepsilon(r_a,x)} \times N_r^{1/3} + a_2 \times \frac{\varepsilon_o(x)}{\varepsilon(r_a,x)} \times N_r^{\frac{1}{3}} \times \left(2.503 \times [-E_{cp}(r_{sp}) \times r_{sp}]\right) + a_3 \times \left[\frac{\varepsilon_o(x)}{\varepsilon(r_a,x)}\right]^{5/4} \times \sqrt{\frac{m_c}{m_v}} \times N_r^{1/4} + 2a_4 \times \sqrt{\frac{\varepsilon_o(x)}{\varepsilon(r_a,x)}} \times N_r^{1/2} + a_5 \times \left[\frac{\varepsilon_o(x)}{\varepsilon(r_a,x)}\right]^{\frac{3}{2}} \times N_r^{\frac{1}{6}}, \quad N_r \equiv \left(\frac{N_a}{9.999 \times 10^{17}\ cm^{-3}}\right), \quad (14p)$$

where $a_1 = 3.15 \times 10^{-3}(eV)$, $a_2 = 5.41 \times 10^{-4}(eV)$, $a_3 = 2.32 \times 10^{-3}(eV)$, $a_4 = 4.12 \times 10^{-3}(eV)$ and

$a_5 = 9.80 \times 10^{-5}(eV)$.

So, in the HD[d(a)- $X(x)$- alloy] ER, the effective extrinsic carrier concentration, $n^*_{en(ep)}$, can be defined by:

$$n^*_{en(ep)}\ (N_{d(a)}, T, r_{d(a)}, x) \equiv \sqrt{N_{d(a)} \times p_o(n_o)} = n_{in(ip)}(T, r_{d(a)}, x) \times exp\left[\frac{\Delta E_{agn(agp)}}{2k_BT}\right], \quad (15)$$

where the apparent band gap narrowing (ABGN), $\Delta E_{agn(agp)}$, is given by:

$$\Delta E_{agn}(N_d, T, r_d, x) \equiv \Delta E_{gn}(N_d, r_d, x) + k_BT \times ln\left(\frac{N_d}{N_c(T,x)}\right) - E_{Fn}(N_d, T, x), \quad (16n)$$

$$\Delta E_{agp}(N_a, T, r_a, x) \equiv \Delta E_{gp}(N_a, r_a, x) + k_BT \times ln\left(\frac{N_a}{N_v(T,x)}\right) + E_{Fp}(N_a, T, x)]. \quad (16p)$$

Total Minority-Carrier Saturation Current Density

In the two $n^+(p^+) - p(n)$ [X(x)≡ $Si_{1-x}Ge_x$]- alloy -junction solar cells, denoted respectively by I(II), the total carrier-minority saturation current density is defined by:

$$J_{oI(oII)} \equiv J_{Eno(Epo)} + J_{Bpo(Bno)} \quad (17)$$

where $J_{Bpo(Bno)}$ is the minority-electron (hole) saturation current density injected into the LD[a(d)- $X(x)$- alloy] BR, and $J_{Eno(Epo)}$ is the minority-hole (electron) saturation-current density injected into the HD[d(a)- $X(x)$- alloy] ER.

$J_{Bpo(Bno)}$ in the LD[p(n) type $X(x)$- alloy]BR

Here, $J_{Bpo(Bno)}$ is determined by (Van Cong, 2023):

$$J_{Bpo(Bno)}(N_{a(d)}, T, r_{a(d)}, x) = \frac{e \times n^2_{ip(in)}(T, r_{a(d)}, x) \times \sqrt{\frac{D_{e(h)}(N_{a(d)}, T, r_{a(d)}, x)}{\tau_{eB(hB)}(N_{a(d)})}}}{N_{a(d)}}, \quad (18)$$

where $n_{ip(in)}^2(T, r_{d(a)}, x)$ is determined Eq. (10), $D_{e(h)}(N_{a(d)}, T, r_{a(d)}, x)$ is the minority electron (minority hole) diffusion coefficient:

$$D_e(N_a, T, r_a, x) = \frac{k_B T}{e} \times \left[92 + \frac{1268}{1+\left(\frac{N_a}{1.3\times10^{17} cm^{-3}}\right)^{0.91}}\right] \times \left(\frac{\varepsilon(r_a,x)}{\varepsilon_o(x)}\right)^2 \ (cm^2 s^{-1}), \quad (19a)$$

$$D_h(N_d, T, r_d, x) = \frac{k_B T}{e} \times \left[130 + \frac{370}{1+\left(\frac{N_d}{8\times10^{17}\ cm^{-3}}\right)^{1.25}}\right] \times \left(\frac{\varepsilon(r_d,x)}{\varepsilon_o(x)}\right)^2 \ (cm^2 s^{-1}), \quad (19b)$$

and $\tau_{eB(hB)}(N_{a(d)})$ is the minority electron (minority hole) lifetime in the BR:

$$\tau_{eB}(N_a)^{-1} = \frac{1}{2.5\times10^{-3}} + 3 \times 10^{-13} \times N_a + 1.83 \times 10^{-31} \times N_a^2, \quad (20a)$$

$$\tau_{hB}(N_d)^{-1} = \frac{1}{2.5\times10^{-3}} + 11.76 \times 10^{-13} \times N_d + 2.78 \times 10^{-31} \times N_d^2. \quad (20b)$$

$J_{Eno(Epo)}$ in the HD[n(p) type $X(x)$-alloy]ER

In the non-uniformly and heavily doped emitter region of n(p) type X(x)-devices, the effective Gaussian d(a)-density profile or the d(a) (majority-e(h)) density, is defined in such the HD[n(p) type $X(x)$-alloy] ER-width W, as (Van Cong, 2023; Van Cong et al., 2023):

$$\rho_{d(a)}(y, N_{d(a)}, W) = N_{d(a)} \times exp\left\{-\left(\frac{y}{W}\right)^2 \times ln\left[\frac{N_{d(a)}}{N_{do(ao)}(W)}\right]\right\} \equiv N_{d(a)} \times \left[\frac{N_{d(a)}}{N_{do(ao)}(W)}\right]^{-\left(\frac{y}{W}\right)^2}, \quad 0 \le y \le W,$$

$$N_{do(ao)}(W) \equiv 7.9 \times 10^{17}(2 \times 10^5) \times exp\left\{-\left(\frac{W}{184.2\ (1)\times10^{-7}\ cm}\right)^{1.066\ (0.5)}\right\} \ (cm^{-3}), \quad (21)$$

where $\rho_{d(a)}(y = 0) = N_{d(a)}$ is the surface d(a)-density, and at the emitter-base junction, $\rho_{d(a)}(y = W) = N_{do(ao)}(W)$, which decreases with increasing W. Further, the "effective doping density" is defined by:

$$N_{d(a)}^*(y, N_{d(a)}, T, r_{d(a)}, x) \equiv \rho_{d(a)}(y)/exp\left[\frac{\Delta E_{agn(agp)}(\rho_{d(a)}, T, r_{d(a)}, x)}{k_B T}\right],$$

$$N_{d(a)}^*(y = 0, N_{d(a)}, T, r_{d(a)}, x) \equiv \frac{N_{d(a)}}{exp\left[\frac{\Delta E_{agn(agp)}(N_{d(a)}, T, r_{d(a)}, x)}{k_B T}\right]}, \text{ and}$$

$$N_{d(a)}^*(y = W, T, r_{d(a)}, x) \equiv \frac{N_{do(ao)}(W)}{exp\left[\frac{\Delta E_{agn(agp)}(N_{do(ao)}(W), T, r_{d(a)}, x)}{k_B T}\right]}, \quad (22)$$

where the apparent band gap narrowing $\Delta E_{agn(agp)}$ is determined in Eq. (16), replacing $N_{d(a)}$ by $\rho_{d(a)}\left(y, N_{d(a)}, W\right)$.

Now, we can define the minority hole (minority electron) transport parameter $F_{h(e)}$ as:

$$F_{h(e)}(y, N_{d(a)}, T, r_{d(a)}, x) \equiv \frac{n_{in(ip)}^2(T, r_{d(a)})}{p_o(n_o) \times D_{h(e)}} = \frac{N_{d(a)}^*}{D_{h(e)}} \equiv \frac{N_{d(a)}}{D_{h(e)}} \times \left(\frac{n_{in(ip)}}{n_{in(ip)}^*}\right)^2 \equiv \frac{N_{d(a)}}{D_{h(e)} \times exp\left[\frac{\Delta E_{agn(agp)}}{k_B T}\right]} \; (cm^{-5} \times s), \quad (23)$$

the minority hole (electron) diffusion length, $L_{h(e)}\left(y, N_{d(a)}, T, r_{d(a)}, x\right)$ by:

$$L_{h(e)}^{-2}\left(y, N_{d(a)}, T, r_{d(a)}, x\right) = \left[\tau_{hE(eE)} \times D_{h(e)}\right]^{-1} = \left(C \times F_{h(e)}\right)^2 = \left(C \times \frac{N_{d(a)}^*}{D_{h(e)}}\right)^2 = \left(C \times \frac{n_{in(ip)}^2(T, r_{d(a)})}{p_o(n_o) \times D_{h(e)}}\right)^2,$$

where the constant C was chosen to be equal to: $2.0893 \times 10^{-30}\; (cm^4/s)$, and the minority hole (minority electron) lifetime $\tau_{hE(eE)}$ as:

$$\tau_{hE(eE)} \equiv \frac{1}{D_{h(e)} \times L_{h(e)}^{-2}} = \frac{1}{D_{h(e)} \times \left(C \times F_{e(h)}\right)^2}. \quad (24)$$

Then, under low-level injection, in the absence of external generation, and for the steady-state case, we can define the minority-h(e) density by:

$$p_o(y)[n_o(y)] \equiv \frac{n_{in(ip)}^2}{N_{d(a)}^*(y=W, T, r_{d(a)}, x)}, \quad (25)$$

and a normalized excess minority-h(e) density u(x) or a relative deviation between $p(y)[n(y)]$ and $p_o(y)[n_o(y)]$.

$$u(y) \equiv \frac{p(y)[n(y)] - p_o(y)[n_o(y)])}{p_o(y)[n_o(y)]}, \quad (26)$$

which must verify the two following boundary conditions as:

$$u(y=0) \equiv \frac{-J_h(y=0)[J_e(y=0)]}{eS \times p_o(y=0)[n_o(y=0)]},$$

$$u(y=W)=exp\left(\frac{V}{n_{I(II)}(V)\times V_T}\right)-1.$$

Here, $n_{I(II)}(V)$ *is* the photovoltaic conversion factor, being determined later, $S\left(\frac{cm}{s}\right)$ is the 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 (electron) current density $J_{h(e)}\left(y, r_{d(a)}, x\right)$.

Further, from the Fick's law for minority hole (electron)-diffusion equations, one has (Van Cong et al., 2023; Van Cong, 2023):

$$J_{h(e)}\left(y, r_{d(a)}, x\right)=\frac{-e(+e)\times n_{in(ip)}^2}{F_{h(e)}(y)}\times\frac{du(y)}{dy}=\frac{-e(+e)n_{in(ip)}^2 D_{h(e)}(N_{d(a)}, r_{d(a)}, x)}{N_{d(a)}^*(y, r_{d(a)}, x)}\times\frac{du(y)}{dy}, \quad (27)$$

where $N_{d(a)}^*(y, r_{d(a)}, x)$ is given in Eq. (22), $D_{h(e)}$ and $F_{h(e)}$ are determined respectively in Equations (19) and (23), and from the minority-hole (electron) continuity equation as:

$$\frac{dJ_{h(e)}(y, r_{d(a)}, x)}{dy}=-e(+e)\times n_{i\,n(p)}^2\times\frac{u(y)}{F_{h(e)}(y)\times L_{h(e)}^2(y)}=-e(+e)\times n_{i\,n(p)}^2\times\frac{u(y)}{N_{d(a)}^*(y, r_{d(a)}, x)\times\tau_{hE(eE)}}, \quad (28)$$

Therefore, the following second-order differential equation is obtained:

$$\frac{d^2u(y)}{dy^2}-\frac{dF_{h(e)}(y)}{dy}\times\frac{du(y)}{dy}-\frac{u(y)}{L_{h(e)}^2(y)}=0, \quad (29)$$

Then, taking into account the two above boundary conditions given in Eq. (22), one thus gets the general solution of this Eq. (29), as:

$$u(y)=\frac{sinh(P(y))+I(W,S)\times cosh(P(y))}{sinh(P(W))+I(W,S)\times cosh(P(W))}\times\left(exp\left(\frac{V}{n_{I(II)}(V)\times V_T}\right)-1\right), \quad (30)$$

where the factor $I(W,S)$ is determined by: $D_{h(e)}\left(N_d, T, r_{d(a)}, x\right)$

$$I(T, r_{d(a)}, x, W, S)=\frac{D_{h(e)}(y=W, N_{do(ao)}(W), T, r_{d(a)}, x)}{S\times L_{h(e)}(y=W, N_{do(ao)}(W), T, r_{d(a)}, x)}. \quad (31)$$

Further, since $\frac{dP(y)}{dy}\equiv C\times F_{h(e)}(y)=\frac{1}{L_{h(e)}(x)}$, $C=2.0893\times 10^{-30}\ (cm^4/s)$, for the X(x)-alloy, being an empirical parameter, chosen for each crystalline semiconductor, P(y) is thus found to be defined by:

$$P(y) \equiv \int_0^y \frac{dy}{L_{h(e)}(y)}), \qquad 0 \le y \le W, \qquad P(y=W) \equiv (\frac{1}{W} \times \int_0^W \frac{dy}{L_{h(e)}(y)}) \times W \equiv \frac{W}{L^*_{h(e)}(y)} = \frac{L_{h(e)}(y)}{L^*_{h(e)}(y)} \times \frac{W}{L_{h(e)}(y)}, \tag{32}$$

where $L^*_{h(e)}(y)$ is the effective minority hole (minority electron) diffusion length. Further, the minority-hole (electron) current density injected into the HD[d(a)- X(x) alloy] ER is found to be given by:

$$J_{h(e)}(y, W, N_{d(a)}, T, r_{d(a)}, x, S, V) = -J_{Eno}(y, W, N_d, T, r_d, x, S)\, [J_{Epo}(y, W, N_a, T, r_a, x, S)] \times \left(exp\left(\frac{V}{n_{I(II)}(V) \times V_T}\right) - 1\right), \tag{33}$$

where $J_{Eno(Epo)}$ is the saturation minority-hole (minority-electron) current density,

$$J_{Eno(Epo)}(y, W, N_{d(a)}, T, r_{d(a)}, x, S) = \frac{en^2_{in(ip)} \times D_{h(e)}}{N^*_{d(a)}(y, N_{d(a)}, T, r_{d(a)}, x) \times L_{h(e)}} \times \frac{cosh(P(x)) + I(W,S) \times sinh(P(x))}{sinh(P(W)) + I(W,S) \times cosh(P(W))}. \tag{34}$$

In the following, we will denote P(W) and $I(W,S)$ by P and I, for a simplicity. So, Eq. (30) gives:

$$J_{Eno(Epo)}(y=0, W, N_{d(a)}, T, r_{d(a)}, x, S) = \frac{en^2_{in(ip)} \times D_{h(e)}}{N^*_{d(a)}(y, N_{d(a)}, T, r_{d(a)}, x) \times L_{h(e)}} \times \frac{1}{sinh(P) + I \times cosh(P)}, \tag{35}$$

$$J_{Eno(Epo)}(y=W, W, N_{d(a)}, T, r_{d(a)}, x, S) = \frac{en^2_{i\,n(ip)} \times D_{h(e)}}{N^*_{d(a)}(y=W, N_{d(a)}, T, r_{d(a)}, x) \times L_{h(e)}} \times \frac{cosh(P) + I \times sinh(P)}{sinh(P) + I \times cosh(P)}, \tag{36}$$

and then,

$$\frac{J_{h(e)}(y=0, W, N_{d(a)}, T, r_{d(a)}, x, S, V)}{J_{h(e)}(y=W, W, N_{d(a)}, T, r_{d(a)}, x, S, V)} \equiv \frac{J_{Eno(Epo)}(y=0, W, N_{d(a)}, T, r_{d(a)}, x, S)}{J_{Eno(Epo)}(y=W, W, N_{d(a)}, T, r_{d(a)}, x, S)} = \frac{1}{cosh(P) + I \times sinh(P)}. \tag{37}$$

Now, if defining the effective excess minority-hole (electron) charge storage in the emitter region by:

$$Q^*_{h(e)}(y=W, N_{d(a)}, T, r_{d(a)}, x) \equiv \int_0^W +e(-e) \times u(y) \times p_o(y)[n_o(y)] \times \frac{\tau_{hE(eE)}(N_{d(a)}, T, r_{d(a)}, x)}{\tau_{hE(eE)}(\rho_{d(a)}(x), T, r_{d(a)}, x)}\, dy,$$

and the effective minority hole (minority electron) transit time $[htt(ett)]$ by: $\tau^*_{htt(ett)}(y =$

$W,W,N_{d(a)},r_{d(a)},x,S) \equiv Q^{*}_{h(e)}(y=W,N_{d(a)},T,r_{d(a)},x)/J_{Eno(Epo)}\big(y=$
$W,W,N_{d(a)},T,r_{d(a)},x,S\big)$, and from Equations (24, 31), one obtains:

$$\frac{\tau^{*}_{htt(ett)}\big(y=W,W,N_{d(a)},T,r_{d(a)},x,S\big)}{\tau_{hE(eE)}} \equiv 1-\frac{J_{Eno(Epo)}\big(y=0,W,N_{d(a)},T,r_{d(a)},x,S\big)}{J_{Eno(Epo)}\big(y=W,W,N_{d(a)},T,r_{d(a)},x,S\big)} = 1-\frac{1}{cosh(P)+I\times sinh(P)}. \quad (38)$$

Now, some important results can be obtained and discussed below.

As $P \ll 1$ (or $W \ll L_{h(e)}$) and $S \to \infty$, $I \equiv I(W,S) = \frac{D_{h(e)}(N_{do(ao)}(W),T,r_{d(a)},x)}{S\times L_{h(e)}(N_{do(ao)}(W),T,r_{d(a)},x)} \to 0$, from Eq. (38), one has: $\frac{\tau^{*}_{htt(ett)}\big(y=W,W,N_{d(a)},T,r_{d(a)},x,S\big)}{\tau_{hE(eE)}} \to 0$, suggesting a completely transparent emitter region (CTER)-case, where, from Eq. (36), one obtains:

$$J_{Eno(Epo)}\big(y=W,N_{d(a)},T,r_{d(a)},x,S\to\infty\big) \to \frac{en^{2}_{in(ip)}\times D_{h(e)}}{N^{*}_{d(a)}(y=W,N_{d(a)},T,r_{d(a)},x)\times L_{h(e)}} \times \frac{1}{P(W)}. \quad (39)$$

Further, as $P \gg 1$ (or $W \gg L_{h(e)}$) and $S \to 0$, $I \equiv I(y=W,r_{d(a)},x,S) = \frac{D_{h(e)}(N_{do(ao)}(W),T,r_{d(a)},x)}{S\times L_{h(e)}(N_{do(ao)}(W),T,r_{d(a)},x)} \to \infty$, and from Eq. (38) one has: $\frac{\tau^{*}_{htt(ett)}\big(y=W,W,N_{d(a)},T,r_{d(a)},x,S\big)}{\tau_{hE(eE)}} \to 1$, suggesting a completely opaque emitter region (COER)-case, where, from Eq. (36), one gets:

$$J_{Eno(Epo)}\big(y=W,N_{d(a)},T,r_{d(a)},x,S\to 0\big) \to \frac{en^{2}_{in(ip)}\times D_{h(e)}}{N^{*}_{d(a)}(y=W,N_{d(a)},T,r_{d(a)},x)\times L_{h(e)}} \times tanh(P). \quad (40)$$

In summary, in the two $n^{+}(p^{+})-p(n)$ X(x)-alloy junction solar cells, the dark carrier-minority saturation current density $J_{oI(oII)}$, defined in Eq. (17), is now rewritten as:

$$J_{oI(oII)}\big(W,N_{d(a)},T,r_{d(a)},x,S;\ N_{a(d)},r_{a(d)},x\big) \equiv J_{Eno(Epo)}(W,N_{d(a)},T,r_{d(a)},x,S) + J_{Bpo(Bno)}(N_{a(d)},T,r_{a(d)},x), \quad (41)$$

where $J_{Eno(Epo)}$ and $J_{Bpo(Bno)}$ are determined respectively in Equations (36, 18).

Photovoltaic conversion effect at 300K

Here, in the $n^{+}(p^{+})-p(n)$ [$X(x)\equiv Si_{1-x}Ge_{x}$] -alloy junction solar cells at T=300 K, denoted respectively by I(II), and for physical conditions, respectively, as:

$$W = 15\ \mu m, N_{d(a)} = 10^{20}\ cm^{-3}, r_{d(a)}, x, S = 100\ \left(\frac{cm}{s}\right);\ N_{a(d)} = 10^{17}\ cm^{-3}, r_{a(d)}, x, \quad (42)$$

we propose, at given open circuit voltages: $V_{ocI1(ocI2)}$ and $V_{ocII1(ocII2)}$, the corresponding data of the short circuit current density $J_{scI(II)}$, in order to formulate our following treatment method of two fix points (Green, 2022; Moon et al., 2016), as:

$$\text{at } V_{ocI1(ocI2)}(V) = 0.624\ (0.740),\ J_{scI1(scI2)}(mA/cm^2) = 36.3\ (41.88),$$
$$\text{at } V_{ocII1(ocII2)}(V) = 0.639\ (0.738)\ ,\ J_{scII1(scII2)}(mA/cm^2) = 39.3\ (42.6). \quad (43)$$

Now, we define the net current density J at T=300 K, obtained for the infinite shunt resistance, and expressed as a function of the applied voltage V, flowing through the $n^+(p^+) - p(n)$ X(x)-alloy junction of solar cells, as:

$$J(V) \equiv J_{ph.}(V) - J_{oI(oII)} \times \left(e^{X_{I(II)}(V)} - 1\right),\ X_{I(II)}(V) \equiv \frac{V}{n_{I(II)}(V) \times V_T},\ \ V_T \equiv \frac{k_B T}{e} = 0.02585\ V, \quad (44)$$

where the function $n_{I(II)}(V)$ is the photovoltaic conversion factor (PVCF), noting that as $V = V_{oc}$, being the open circuit voltage, $J(V = V_{oc}) = 0$, the photocurrent density is defined by: $J_{ph.}(V = V_{oc}) \equiv J_{scI(scII)}\left(W, N_{d(a)}, T, r_{d(a)}, x, S;\ N_{a(d)}, T, r_{a(d)}, x, V_{oc}\right)$, for $V_{oc} \geq V_{ocI1(ocII1)}$.

Therefore, the photovoltaic conversion effect occurs, according to:

$$J_{scI(scII)}\left(W, N_{d(a)}, T, r_{d(a)} x, S;\ N_{a(d)}, T, r_{a(d)}, x, V_{oc}\right) \equiv J_{oI(oII)}\left(W, N_{d(a)}, T, r_{d(a)}, x, S;\ N_{a(d)}, T, r_{a(d)}, x\right) \times \left(e^{X_{I(II)}(V_{oc})} - 1\right), \quad (45)$$

where $n_{I(II)}(V_{oc}) \equiv n_{I(II)}\left(W, N_{d(a)}, T, r_{d(a)}, x, S;\ N_{a(d)}, r_{a(d)}, x, V_{oc}\right)$, and $X_{I(II)}(V_{oc}) \equiv \frac{V_{oc}}{n_{I(II)}(V_{oc}) \times V_T}$.

Here, one remarks that (i) for a given V_{oc}, both $n_{I(II)}$ and $J_{oI(II)}$ have the same variations, obtained in the same physical conditions, as observed in the following calculation, (ii) the function $\left(e^{X_{I(II)}(V_{oc})} - 1\right)$ [or the PVCF, $n_{I(II)}$], representing the photovoltaic conversion effect, converts the light, represented by $J_{scI(scII)}$, into the electricity, by $J_{oI(oII)}$, and finally, for given $\left(W, N_{d(a)}, T, r_{d(a)}, x, S;\ N_{a(d)}, T, r_{a(d)}, x, V_{oc}\right)$-values, $n_{I(II)}(V_{oc})$ is determined.

Now, for $V_{oc} \geq V_{ocI1(ocII1)}$, one can propose the general expressions for the PVCF, in order to get exactly the values of $n_{I1(II1)}\left(V_{ocI1(ocII1)}\right)$ and $n_{I2(II2)}\left(V_{ocI2(ocII2)}\right)$, as functions of V_{oc}, by:

$$n_{I(II)}\left(W, N_{d(a)}, T, r_{d(a)}, x, S;\ N_{a(d)}, T, r_{a(d)}, x, V_{oc}\right) = n_{I1(II1)}\left(V_{ocI1(ocII1)}\right) + n_{I2(II2)}\left(V_{ocI2(ocII2)}\right) \times \left(\frac{V_{oc}}{V_{ocI1(ocII1)}} - 1\right)^{\alpha(\beta)}, \quad (46)$$

where, the values of $\alpha(\beta)$, obtained for $x = (0, 0.5, \text{and } 1)$, will be reported in next Tables 3 and 5. One also notes that those $\alpha(\beta)$-values depend on $(W, N_{d(a)}, T, r_{d(a)}, x, S;\ N_{a(d)}, T, r_{a(d)}, x)$-ones.

So, one can determine the general expressions for the fill factors, as:

$$F_{I(II)}\left(W, N_{d(a)}, T, r_{d(a)}, x, S; N_{a(d)}, T, r_{a(d)}, x, V_{oc}\right) = \frac{X_{I(II)}(V_{oc}) - \ln[X_{I(II)}(V_{oc}) + 0.72]}{X_{I(II)}(V_{oc}) + 1}. \quad (47)$$

Finally, the efficiency $\eta_{I(II)}$ can be defined in the $n^{+}(p^{+}) - p(n)$ X(x) alloy-junction solar cells, by:

$$\eta_{I(II)}\left(W, N_{d(a)}, T, r_{d(a)}, x, S;\ N_{a(d)}, T, r_{a(d)}, x, V_{oc}\right) \equiv \frac{J_{scI(scII)} \times V_{oc} \times F_{I(II)}}{P_{in.}}, \quad (48)$$

being assumed to be obtained at 1 sun illumination or at AM1.5G spectrum ($P_{in.} = 0.100\ \frac{W}{cm^2}$).

It should be noted that the maximal values of $\eta_{I(II)}$, $\eta_{Imax.(IImax.)}$, are obtained at the corresponding ones of $V_{oc} = V_{ocI(ocII)}$, at which $\left(\frac{\partial \eta_{I(II)}(W, N_{d(a)}, T, r_{d(a)}, S, N_{a(d)}, r_{a(d)}, V_{oc})}{\partial V_{oc}}\right)_{V_{oc} = V_{ocI(ocII)}} = 0$, as those given in next Tables 3 and 4, being marked in bold. Further, from the well-known Carnot's theorem, being obtained by the entropy law, the maximum efficiency of a heat engine operating between hot (H) and cold (C) reservoirs is the ratio of the temperature difference between the reservoirs, $T_H - T_C$, $T_C \equiv T = 300$ K, to the H-reservoir temperature, T_H, expressed as:

$$\eta_{I(II)}(T, V_{oc}) \leq \eta_{Imax.(IImax.)}\left(T, V_{oc} = V_{ocI(ocII)}\right) \equiv \eta_{Carnot} = \frac{T_H - T_C}{T_H}, \quad (49)$$

for a simplicity, noting that both $\eta_{Imax.(IImax.)}$ and T_H depend on $(W, N_{d(a)}, T, r_{d(a)}, S, N_{a(d)}, r_{a(d)}, V_{ocI(ocII)})$-parameters.

Numerical Results and Concluding Remarks

We will respectively consider the two following cases of $n^{+}(p^{+}) - p(n)$ -junctions such as:

HD (Te ; Sb; Sn) X(x) − alloy ER − LD (Mg ; In ; Cd) X(x)] − alloy BR −case, according to: 3 $(n^{+}p)$ − junctions denoted by: $(Te^{+}Mg, Sb^{+}In, Sn^{+}Cd)$, and

HD (Mg ; In ; Cd) X(x) − alloy ER − LD (Te; Sb; Sn) X(x) − alloy BR −case, according to: 3 $(p^{+}n)$ − junctions denoted by: $(Mg^{+}Te, In^{+}Sb, Cd^{+}Sn)$.

Now, by using the physical conditions, given in Eq. (42), then, if denoting: heavily doped (HD), lightly doped (LD), emitter region (ER), and base region (BR), we can determine various photovoltaic conversion coefficients, as follows.

Firs case: HD [Te; Sb; Sn] X(x) − Alloy ER − LD [Mg ; In ; Cd] X(x) − Alloy BR

Here, there are the 3 $(n^+p) - X(x)$ junctions, being denoted by: (Te^+Mg, Sb^+In, Sn^+Cd).

Then, the numerical results of $\frac{\tau^*_{htt}}{\tau_{hE}}$, J_{Bpo}, J_{Eno} and J_{oI}, are calculated, using Equations (38), (18), (36) and (41), respectively, and reported in Table 2, in which J_{oI} decreases slightly with increasing $r_{d(a)}$-radius for given x, but it increases strongly with increasing x for given $r_{d(a)}$-radius. Further, those of n_I, J_{scI}, F_I, η_I, and T_H, are computed, using Equations (46, 45, 47, 48, 49), respectively, and reported in Table 3.

Tables 2 and 3 in Appendix 1

Second case: HD [Mg ; In ; Cd] X(x) − Alloy ER − LD [Te; Sb, Sn] X(x) − Alloy BR

Here, there are 3 $(p^+n) - X(x)$-junctions, being denoted by: (Mg^+Te, In^+Sb, Cd^+Sn).

Then, the numerical results of $\frac{\tau^*_{ett}}{\tau_{eE}}$, J_{Bno}, J_{Epo} and J_{oII}, are calculated using Equations (38), (18), (36) and (41), respectively, and reported in Table 4, in which J_{oII} decreases slightly with increasing $r_{a(d)}$-radius for given x, but it increases strongly with increasing x for given $r_{a(d)}$-radius. Further, those of n_{II}, J_{scII}, F_{II}, η_{II}, and T_H, are computed, using Equations (46, 45, 47, 48, 49), respectively, and reported in Table 5.

Tables 4 and 5 in Appendix 1

Finally, some concluding remarks are obtained and discussed in the following.

(i)-First, in the single $n^+ - p$ $Si_{1-x}Ge_x$-alloy junction solar cell, from Table 3, with increasing x=(0, 0.5, 1) and for given $r_{Sn(Cd)}$-radius, for example, one obtains: $\eta_{Imax.}$(↘)= **28.21%**, 25.97%, **23.36%**, according to $T_H(K) = \mathbf{417.9}, 405.2, \mathbf{391.4}$, at $V_{ocI}(V) = \mathbf{0.70}, 0.71, \mathbf{0.74}$, noting that the values, marked in bold, correspond to those obtained respectively for x=(0, 1).

(ii)- Secondly, in the single $p^+ - n$ $Si_{1-x}Ge_x$-alloy junction solar cell, from Table 5, with increasing x=(0, 0.5, 1) and for given $r_{Cd(Sn)}$-radius, for example, one obtains: $\eta_{IImax.}$(↘)= **27.66%**, 25.89%, **23.63%**, according to $T_H(K) = \mathbf{414.7}, 404.8, \mathbf{392.8}$, at $V_{ocI}(V) = \mathbf{0.71}, 0.72, \mathbf{0.76}$, noting that the values, marked in bold, correspond to those obtained respectively for x=(0, 1).

(iii)- Then, as noted in (i) and (ii), for x=0, $\eta_{I(II)max.} = 28.21\ \%\ (27.66\ \%)$, which can be compared with

the corresponding ones, 27.19 % and 26.7 %, obtained, for the single-junction Si crystalline solar cell, by Singh and Ravindra (2012) and by Green et al. (2022), respectively.

(iv)- Further, as noted in (i) and (ii), for x=1, $\eta_{I(II)max.} = 23.36\%\ (23.63\%)$, which can be compared with the corresponding ones, 12.50 % and 14.82 %, obtained, for the single-junction Ge crystalline solar cell, by Singh and Ravindra (2012) and by Van Cong (2023), respectively.

Finally, as discussed in above remarks (iii) and (iv), in order to obtain the highest efficiencies, the present single $Si_{1-x}Ge_x$-alloy junction solar cells could be chosen rather than the single crystalline (Si, Ge)-junction solar cells.

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Appendix 1

Table 1 From Equations (5, 8a, 8b, 9) and in the n(p)-type $[X(x) \equiv Si_{1-x}Ge_x]$-alloy, the numerical results of the energy-band-structure parameters, reported below, suggest that: (i) for given x and with increasing $r_{d(a)}$, $\varepsilon(r_{d(a)}, x)$ decreases, while other ones increase, and (ii) for given $r_{d(a)}$ and with increasing x, $E_{gin(gip)}(T = 300K, r_{d(a)}, x)$ decreases

Donor		**Si**	Te	Sb	Sn
r_d (nm)	↗	**r_{do}=0.117**	0.132	0.136	0.140
x	↗	0, 0.5, 1	0, 0.5, 1	0, 0.5, 1	0, 0.5, 1
$B_{do}(x)$ in 10^8 (N/m^2)	↗	8.04, 3.88, 1.56			
$\varepsilon(r_d, x)$	↘	**11.4**, 13.6, **15.8**	10.6, 12.6, 14.7	10.2, 12.1, 14.1	9.69, 11.6, 13.4
$E_d(r_d, x)$ meV	↗	33.7, 16.2, 6.54	39.0, 18.8, 7.57	42.3, 20.4, 8.22	46.6, 22.5, 9.05
$E_{gn}(r_d, x)$ eV	↗	**1.17**, 0.95, **0.74**	1.175, 0.96, 0.742	1.179, 0.960, 0.743	1.183, 0.962, 0.744
$E_{gin}(T = 300K, r_d, x)$ eV	↗	**1.12**, 0.89, **0.66**	1.130, 0.895, 0.662	1.133, 0.897, 0.662	1.138, 0.899, 0.663
Acceptor		**Si**	Mg	In	Cd
r_a (nm)	↗	**r_{ao}=0.117**	0.140	0.144	0.148
x	↗	0, 0.5, 1	0, 0.5, 1	0, 0.5, 1	0, 0.5, 1
$B_{ao}(x)$ in 10^8 (N/m^2)	↗	9.16, 5.85, 3.90			
$\varepsilon(r_a, x)$	↘	**11.4**, 13.6, **15.8**	9.69, 11.6, 13.4	9.19, 10.9, 12.7	8.69, 10.4, 12.0
$E_a(r_a, x)$ meV	↗	38.3, 24.5, 16.3	53.1, 33.9, 22.6	59.0, 37.7, 25.1	66.0, 42.2, 28.1
$E_{gp}(r_a, x)$ eV	↗	**1.17**, 0.95, **0.74**	1.185, 0.96, 0.747	1.191, 0.969, 0.75	1.198, 0.973, 0.753
$E_{gip}(T = 300K, r_a, x)$ eV	↗	**1.12**, 0.89, **0.66**	1.139, 0.90, 0.667	1.145, 0.906, 0.669	1.152, 0.910, 0.672

Table 2. In the HD [(Te; Sb; Sn)- X(x)-alloy] ER-LD[(Mg; In; Cd)-X(x)-alloy] BR, $X(x) \equiv Si_{1-x}Ge_x$, for physical conditions given in Eq. (42) and for a given x, our numerical results of $\frac{\tau^*_{htt}}{\tau_{hE}}$, J_{Bpo}, J_{Eno} and J_{oI}, are computed, using Equations (38), (18), (36) and (41), respectively, noting that J_{oI} decreases slightly with increasing $r_{d(a)}$-radius for given x, but it increases strongly with increasing x for given $r_{d(a)}$-radius, being new results

n^+p		Te^+Mg	Sb^+In	Sn^+Cd
Here, **x=0,** and for the (Te^+Mg, Sb^+In, Sn^+Cd)-junctions and from Eq. (34), one obtains: $\frac{\tau^*_{htt}}{\tau_{hE}} = (0,0,0)$ suggesting a completely transparent condition.				
J_{Bpo} in 10^{-15} (A/cm^2)	↘	2.2097	2.0959	1.9810
J_{Eno} in 10^{-17} (A/cm^2)	↘	7.9977	7.4353	6.7717
J_{oI} in 10^{-15} (A/cm^2)	↘	2.2897	2.1703	2.0487
Here, **x=0.5,** and for the (Te^+Mg, Sb^+In, Sn^+Cd)-junctions and from Eq. (34), one obtains: $\frac{\tau^*_{htt}}{\tau_{hE}} = (0,0,0)$ suggesting a completely transparent condition.				
J_{Bpo} in 10^{-11} (A/cm^2)	↘	1.1133	1.0560	0.9981
J_{Eno} in 10^{-14} (A/cm^2)	↘	1.2724	1.2769	1.2810
J_{oI} in 10^{-11} (A/cm^2)	↘	1.1146	1.0573	0.9994
Here, **x=1,** and for the (Te^+Mg, Sb^+In, Sn^+Cd)junctions and from Eq. (34), one obtains: $\frac{\tau^*_{htt}}{\tau_{hE}} = (0,0,0)$ suggesting a completely transparent condition.				
J_{Bpo} in 10^{-8} (A/cm^2)	↘	3.4701	3.2914	3.1109
J_{Eno} in 10^{-15} (A/cm^2)	↘	1.5623	1.6444	1.7514
J_{oI} in 10^{-8} (A/cm^2)	↘	3.4701	3.2914	3.1109

Table 3. In the HD [(Te; Sb; Sn)- X(x)-alloy] ER-LD[(Mg; In; Cd)-X(x)-alloy] BR, $X(x) \equiv Si_{1-x}Ge_x$, for physical conditions given in Eq. (42) and for a given x, our numerical results of n_I, J_{scI}, F_I, η_I, and T_H, are computed, using Equations (46, 45, 47, 48, 49), respectively, noting that (i) n_I decreases slightly with increasing $r_{d(a)}$-radius for given x and V_{oc}, and (ii) both $\eta_{Imax.}$ and T_H, marked in bold, decrease with increasing x for given $r_{d(a)}$

$V_{oc}(V)$	n_I	$J_{scI}(\frac{mA}{cm^2})$	$F_I(\%)$	$\eta_I(\%)$
Here, **x=0**. For the (Te^+Mg, Sb^+In, Sn^+Cd) junctions, the value of α given in Eq. (46) is 1.1166.				
n^+p	$Te^+Mg;\ Sb^+In;\ Sn^+Cd$	$Te^+Mg;\ Sb^+In;\ Sn^+Cd$	$Te^+Mg;\ Sb^+In;\ Sn^+Cd$	$Te^+Mg;\ Sb^+In;\ Sn^+Cd$
0.624	**0.794; 0.793; 0.791**	**36.30**; **36.30**; **36.30**	**85.86**; **85.88**; 85.90	**19.45**; **19.45**; **19.46**
0.69	0.870; 0.869; 0.867	47.49; 47.51; 47.53	85.96; 85.98; 85.99	28.16; 28.18; 28.20
0.70	0.883; 0.882; 0.880	46.83; 46.85; 46.87	85.95; 85.97; 85.99	**28.17**; **28.19**; **28.21**
			$\boldsymbol{V_{ocI} = 0.70\ V}$	**417.6; 417.8; 417.9=$\boldsymbol{T_H(K)}$**
0.71	0.897; 0.895; 0.893	45.88; 45.90; 45.92	85.94; 85.96; 85.98	28.01; 27.97; 28.03
0.74	0.937; 0.936; 0.934	41.88; 41.89; 41.89	85.91; 85.93; 85.95	26.62; 26.64; 26.65
3	4.965; 4.957; 4.947	0.032; 0.032; 0.0321	82.84; 82.86; 82.88	0.080; 0.079; 0.078
Here, **x=0.5**. For the (Te^+Mg, Sb^+In, Sn^+Cd) junctions, the value of α given in Eq. (46) is 1.1225				
n^+p	$Te^+Mg;\ Sb^+In;\ Sn^+Cd$	$Te^+Mg;\ Sb^+In;\ Sn^+Cd$	$Te^+Mg;\ Sb^+In;\ Sn^+Cd$	$Te^+Mg;\ Sb^+In;\ Sn^+Cd$
0.624	**1.102; 1.099; 1.096**	**36.30**; **36.30**; **36.30**	**82.02**; **82.05**; **82.08**	**18.58**; **18.58**; **18.59**
0.70	1.224; 1.221; 1.218	45.01; 45.03; 45.06	82.14; 82.17; 82.21	25.88; 25.90; 25.93
0.71	1.242; 1.239; 1.236	44.45; 44.47; 44.95	82.13; 82.17; 82.20	**25.92; 25.94**; **25.97**
			$\boldsymbol{V_{ocI} = 0.71\ V}$	**404.9; 405.1; 405.2=$\boldsymbol{T_H(K)}$**
0.72	1.261; 1.258; 1.254	43.72; 43.74; 43.75	82.12; 82.16; 82.19	25.85; 25.87; 25.89
0.74	1.298; 1.295; 1.292	41.85; 41.86; 41.87	82.10; 82.13; 82.16	25.42; 25.44; 25.46
3	6.925; 6.909; 6.891	0.211; 0.208; 0.205	78.25; 78.29; 78.33	0.495; 0.489; 0.482
Here, **x=1**. For the (Te^+Mg, Sb^+In, Sn^+Cd) junctions, the value of α given in Eq. (46) is 1.1345				
n^+p	$Te^+Mg;\ Sb^+In;\ Sn^+Cd$	$Te^+Mg;\ Sb^+In;\ Sn^+Cd$	$Te^+Mg;\ Sb^+In;\ Sn^+Cd$	$Te^+Mg;\ Sb^+In;\ Sn^+Cd$
0.624	**1.741; 1.735; 1.728**	**36.30**; **36.30**; **36.30**	**75.24**; **75.30**; **75.37**	**17.04**; **17.06**; **17.07**
0.72	1.986; 1.978; 1.970	42.74; 42.76; 42.79	75.43; 75.50; 75.56	23.21; 23.24; 23.28
0.73	2.015; 2.007; 1.999	42.29; 42.31; 42.34	75.42; 75.48; 75.55	23.28; 23.32; 23.35
0.74	2.044; 2.037; 2.028	41.76; 41.77; 41.79	75.41; 75.47; 75.54	**23.30**; **23.33**; **23.36**
			$\boldsymbol{V_{ocI} = 0.74\ V}$	**391.1; 391.3; 391.4=$\boldsymbol{T_H(K)}$**
0.75	2.074; 2.066; 2.058	41.15; 41.16; 41.18	75.39; 75.45; 75.52	23.26; 23.29; 23.32
3	11.06; 11.02; 10.97	1.251; 1.235; 1.218	70.27; 70.34; 70.41	2.638; 2.606; 2.572

Table 4. In the HD [(Mg; In; Cd)- X(x)-alloy] ER-LD[(Te; Sb; Sn)-X(x)-alloy] BR, $X(x) \equiv Si_{1-x}Ge_x$, for physical conditions given in Eq. (42) and for a given x, our numerical results of $\frac{\tau^*_{ett}}{\tau_{eE}}$, J_{Bno}, J_{Epo}, and J_{oII} are computed, using Equations (38), (18), (36) and (41), respectively, noting that J_{oII} decreases slightly with increasing $r_{a(d)}$-radius for given x, but it increases strongly with increasing x for given $r_{a(d)}$-radius, being new results

p^+n		Mg^+Te	In^+Sb	Cd^+Sn
Here, **x=0,** and for the (Mg^+Te, In^+Sb, Cd^+Sn)-junctions and from Eq. (34), one obtains: $\frac{\tau^*_{ett}}{\tau_{eE}} = (0,0,0)$ suggesting a completely transparent condition.				
J_{Bno} in 10^{-15} (A/cm^2)	↘	4.8309	4.0706	3.2913
J_{Epo} in 10^{-17} (A/cm^2)	↘	3.0212	2.4972	1.9936
J_{oII} in 10^{-15} (A/cm^2)	↘	4.8611	4.0956	3.3113
Here, **x=0.5,** and for the (Mg^+Te, In^+Sb, Cd^+Sn)-junctions and from Eq. (34), one obtains: $\frac{\tau^*_{ett}}{\tau_{eE}} = (0,0,0)$ suggesting a completely transparent condition.				
J_{Bno} in 10^{-11} (A/cm^2)	↘	2.0898	1.8834	1.6583
J_{Epo} in 10^{-14} (A/cm^2)	↘	7.7141	6.9161	6.0826
J_{oII} in 10^{-11} (A/cm^2)	↘	2.0976	1.8903	1.6644
Here, **x=1,** and for the (Mg^+Te, In^+Sb, Cd^+Sn)-junctions and from Eq. (34), one obtains: $\frac{\tau^*_{ett}}{\tau_{eE}} = (0,0,0)$ suggesting a completely transparent condition.				
J_{Bno} in 10^{-8} (A/cm^2)	↘	5.9839	5.5985	5.1687
J_{Epo} in 10^{-10} (A/cm^2)	↘	1.0472	0.9830	0.9133
J_{oII} in 10^{-8} (A/cm^2)	↘	5.9944	5.6083	5.1778

Table 5. In the HD [(Mg; In; Cd)- X(x)-alloy] ER-LD[(Te; Sb; Sn)-X(x)-alloy] BR, $X(x) \equiv Si_{1-x}Ge_x$, for physical conditions given in Eq. (42) and for a given x, our numerical results of n_{II}, J_{scII}, F_{II}, η_{II}, and T_H, are computed, using Equations (46, 45, 47, 48, 49), respectively, noting that (i) n_{II} decreases slightly with increasing $r_{a(d)}$-radius for given x and V_{oc}, and (ii) both $\eta_{IImax.}$ and T_H, marked in bold, decrease with increasing x for given $r_{a(d)}$

$V_{oc}(V)$	n_{II}	$J_{scII}(\frac{mA}{cm^2})$	$F_{II}(\%)$	$\eta_{II}(\%)$
Here, **x=0**. For the (Mg^+Te, In^+Sb, Cd^+Sn)-junctions, the value of β given in Eq. (46) is 1.0866.				
p^+n	$Mg^+Te;\ In^+Sb;\ Cd^+Sn$	$Mg^+Te;\ In^+Sb;\ Cd^+Sn$	$Mg^+Te;\ In^+Sb;\ Cd^+Sn$	$Mg^+Te;\ In^+Sb;\ Cd^+Sn$
0.639	0.832; 0.827; 0.821	39.30; 39.30; 39.30	85.63; 85.69; 85.76	21.50; 21.52; 21.54
0.70	0.906; 0.901; 0.895	45.97; 46.00; 46.06	85.68; 85.74; 85.82	27.57; 27.61; 27.67
0.71	0.920; 0.914; 0.908	45.33; 45.36; 45.40	85.68; 85.74; 85.81	**27.57**; 27.61; 27.66
			$\boldsymbol{V_{ocI} = 0.71\ V}$	**414.2; 414.4; 414.7=$\boldsymbol{T_H(K)}$**
0.72	0.933; 0.928; 0.921	44.47; 44.50; 44.54	85.67; 85.73; 85.81	27.43; 27.47; 27.52
0.738	0.958; 0.952; 0.946	42.56; 42.58; 42.60	85.65; 85.72; 85.79	26.90; 26.94; 26.97
3	4.795; 4.767; 4.734	0.157; 0.152; 0.146	83.27; 83.34; 83.43	0.393; 0.381; 0.367
Here, **x=0.5**. For the (Mg^+Te, In^+Sb, Cd^+Sn)-junctions, the value of β given in Eq. (46) is 1.0905.				
p^+n	$Mg^+Te;\ In^+Sb;\ Cd^+Sn$	$Mg^+Te;\ In^+Sb;\ Cd^+Sn$	$Mg^+Te;\ In^+Sb;\ Cd^+Sn$	$Mg^+Te;\ In^+Sb;\ Cd^+Sn$
0.639	1.158; 1.152; 1.145	39.30; 39.30; 39.30	81.68; 81.75; 81.82	20.51; 20.53; 20.55
0.71	1.279; 1.273; 1.265	44.41; 44.43; 44.46	81.76; 81.82; 81.90	25.78; 25.81; 25.85
0.72	1.298; 1.291; 1.284	43.87; 43.89; 43.92	81.75; 81.81; 81.89	**25.82; 25.85; 25.89**
			$\boldsymbol{V_{ocI} = 0.72\ V}$	**404.4; 404.6; 404.8=$\boldsymbol{T_H(K)}$**
0.73	1.317; 1.310; 1.302	43.21; 43.23; 43.25	81.74; 81.80; 81.88	25.78; 25.81; 25.85
0.738	1.332; 1.325; 1.318	42.60; 42.62; 42.64	81.73; 81.79; 81.87	25.70; 25.73; 25.76
3	6.696; 6.664; 6.625	0.703; 0.689; 0.673	78.76; 78.83; 78.92	1.661; 1.630; 1.593
Here, **x=1**. For the (Mg^+Te, In^+Sb, Cd^+Sn)-junctions, the value of β given in Eq. (46) is 1.0369.				
p^+n	$Mg^+Te;\ In^+Sb;\ Cd^+Sn$	$Mg^+Te;\ In^+Sb;\ Cd^+Sn$	$Mg^+Te;\ In^+Sb;\ Cd^+Sn$	$Mg^+Te;\ In^+Sb;\ Cd^+Sn$
0.639	1.845; 1.836; 1.825	39.30; 39.30; 39.30	74.66; 74.74; 74.84	18.75; 18.77; 18.79
0.738	2.118; 2.108; 2.096	42.59; 42.60; 42.62	74.76; 74.85; 74.95	23.50; 23.53; 23.57
0.75	2.155; 2.144; 2.132	42.02; 42.03; 42.05	74.74; 74.83; 74.93	23.55; 23.59; 23.62
0.76	2.186; 2.175; 2.162	41.49; 41.50; 41.51	74.73; 74.81; 74.91	**23.57**; 23.60; 23.63
			$\boldsymbol{V_{ocI} = 0.76\ V}$	**392.5; 392.7; 392.8=$\boldsymbol{T_H(K)}$**
0.77	2.217; 2.206; 2.193	40.93; 40.93; 40.94	74.71; 74.80; 74.90	23.54; 23.57; 23.61
3	10.74; 10.69; 10.63	2.929; 2.891; 2.846	70.81; 70.90; 71.01	6.222; 6.149; 6.062