



**34.18 % (33.80 %)- HIGHEST EFFICIENCIES IN  $\text{CdTe}_{1-x}\text{S}_x$ -ALLOY JUNCTION SOLAR CELLS AT 300 K, ACCORDING TO HIGHEST HOT RESERVOIR TEMPERATURES, 455.8 K (453.2 K), OBTAINED FROM CARNOT-EFFICIENCY THEOREM. (XIV)**

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Article Received on 21/04/2024

Article Revised on 11/05/2024

Article Accepted on 01/06/2024



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### ABSTRACT

In  $n^+(p^+) - p(n)$  [ $\text{X}(x) \equiv \text{CdTe}_{1-x}\text{S}_x$ ]-alloy junction solar cells at  $T=300$  K,  $0 \leq x \leq 1$ , by basing on the same physical model and the same treatment method, as those used in our recent works<sup>[1,2]</sup>, we will also investigate the maximal efficiencies,  $\eta_{\text{Imax.}(I_{\text{Imax.}})}$ , obtained at the open circuit voltage  $V_{\text{oc}} (= V_{\text{ocI(ocII)}}$ ), according to highest hot reservoir temperatures,  $T_{\text{H}}(\text{K})$ , obtained from the Carnot efficiency theorem, which was demonstrated by the use of the entropy law. In the present work, some concluding remarks are given in the following.

(1) In the heavily doped emitter region, the effective density of electrons (holes),  $N^*$ , given in parabolic conduction (valence) bands, expressed as functions of the total dense impurity density,  $N$ , donor

(acceptor)-radius,  $r_{\text{d(a)}}$ , and  $x$ -concentration, is defined in Eq. (9d), as:  $N^*(N, r_{\text{d(a)}}, x) \equiv N - N_{\text{CDn(NDp)}}(r_{\text{d(a)}}, x)$ , where  $N_{\text{CDn(NDp)}}$  is the Mott critical density in the metal-insulator transition, determined in Eq. (9a). Then, we have showed that (i) the origin of such the Mott's criterium, Eq. (9a), is exactly obtained from the reduced effective Wigner-Seitz radius  $r_{\text{sn(sp)}}$ , characteristic of interactions, as given in Equations (9b, 9c), and further (ii)  $N_{\text{CDn(CDp)}}$  is just the density of electrons (holes) localized in the exponential conduction

(valence)-band tail (EBT), as that demonstrated in.<sup>[1]</sup> In this work,  $N$ , given in<sup>[2]</sup>, is now replaced by  $N^*(N, r_{d(a)}, x)$ , representing the heavily doped compensated emitter region.

(2) In Table 3n, for the  $n^+ - p$   $X(x)$  -alloy junction solar cell and for  $r_{Sn(Cd)}$ -radius, one obtains with increasing  $x=(0, 0.5, 1)$ :  $\eta_{II\max.}(^{\circ}) = 26.12\%, 29.91\%, 34.18\%$ , according to  $T_H(^{\circ}) = 406.1\text{ K}, 428.0\text{ K}, 455.8\text{ K}$ , at  $V_{ocI} = 0.82\text{ V}, 0.81\text{ V}, 0.80\text{ V}$ , respectively.

(3) In Table 5p, for the  $p^+ - n$   $X(x)$  -alloy junction solar cell and for  $r_{Cd(Sn)}$ -radius, one obtains with increasing  $x=(0, 0.5, 1)$ :  $\eta_{II\max.}(^{\circ}) = 25.03\%, 29.57\%, 33.80\%$ , according to  $T_H(^{\circ}) = 400.2\text{ K}, 425.9\text{ K}, 453.2\text{ K}$ , at  $V_{ocII} = 0.82\text{ V}, 0.81\text{ V}, 0.80\text{ V}$ , respectively.

**KEYWORDS:** single  $CdTe_{1-x}S_x$  -alloy junction solar cell; photovoltaic conversion factor; photovoltaic conversion efficiency.

## INTRODUCTION

In single  $n^+(p^+) - p(n)$   $X(x) \equiv CdTe_{1-x}S_x$ -alloy junction solar cells at 300 K,  $0 \leq x \leq 1$ , by basing on the same physical model and treatment method, as used in our two recent works<sup>[1,2]</sup>, and also on other ones<sup>[2-11]</sup>, we will investigate the highest (or maximal) efficiencies,  $\eta_{II\max.}(II\max)$ , according to highest hot reservoir temperatures  $T_H(K)$ , obtained from the Carnot- efficiency theorem, being proved by the entropy law.

In the following, we will show that the energy-band-structure parameters, due to the effects of  $x$ -concentration, size impurity, temperature  $T$  and heavy doping, affect strongly the dark (or total) minority-carrier saturation current density and the photovoltaic conversion effect.

## ENERGY BAND STRUCTURE PARAMETERS

### A. Effect of $x$ - concentration

In the  $n^+(p^+) - p(n)$  single  $n^+(p^+) - p(n)$   $X(x)$ -alloy junction at  $T=0$  K, the energy-band-structure parameters<sup>[1]</sup>, are expressed as functions of  $x$ , are given in the following.

(i)-The unperturbed relative effective electron (hole) mass in conduction (valence) bands are given by:

$$\begin{aligned} m_c(x)/m_0 &= 0.197 \times x + 0.095 \times (1 - x), \text{ and} \\ m_v(x)/m_0 &= 0.801 \times x + 0.82 \times (1 - x). \end{aligned} \quad (1)$$

(ii)-The unperturbed relative static dielectric constant of the intrinsic of the single crystalline  $X$ - alloy is found to be defined by:

$$\epsilon_0(x) = 9 \times x + 10.31 \times (1 - x). \quad (2)$$

(iii)-Finally, the unperturbed band gap at 0 K is found to be given by:

$$E_{go}(x) \text{ in eV} = 2.58 \times x + 1.62 \times (1 - x). \quad (3)$$

Therefore, we can define the effective donor (acceptor)-ionization energy, at  $r_{d(a)} = r_{do(ao)} = r_{Te(Cd)} = 0.132 \text{ nm} (0.148 \text{ nm})$ , in absolute values as:

$$E_{do(ao)}(x) = \frac{13600 \times [m_c(v)(x)/m_o]}{[\epsilon_o(x)]^2} \text{ meV}, \quad (4)$$

and then, the isothermal bulk modulus, by:

$$B_{do(ao)}(x) \equiv \frac{E_{do(ao)}(x)}{\left(\frac{4\pi}{3}\right) \times (r_{do(ao)})^3}. \quad (5)$$

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

Here, the effects of  $r_{d(a)}$  and x- concentration affect the changes in all the energy-band-structure parameters, expressed in terms of the effective relative dielectric constant  $\epsilon(r_{d(a)}, x)$ , in the following.

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  $p$ ,  $p_o = 0$ , and for the deformation potential energy (or the strain energy)  $\sigma$ ,  $\sigma_o = 0$ . Further, the two important equations<sup>[9]</sup>, used to determine the  $\sigma$ -variation,  $\Delta\sigma \equiv \sigma - \sigma_o = \sigma$ , are defined by:

$\frac{dp}{dv} = -\frac{B}{v}$  and  $p = -\frac{d\sigma}{dv}$ . giving:  $\frac{d}{dv}\left(\frac{d\sigma}{dv}\right) = \frac{B}{v}$ . Then, by an integration, one gets:

$$[\Delta\sigma(r_{d(a)}, x)]_{n(p)} = B_{do(ao)}(x) \times (V - V_{do(ao)}) \times \ln\left(\frac{V}{V_{do(ao)}}\right) = E_{do(ao)}(x) \times \left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 \geq 0. \quad (6)$$

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 the effective donor (acceptor)-ionization energy  $E_{d(a)}(r_{d(a)}, x)$  in absolute values, obtained in the effective Bohr model, which is represented respectively by:  $\pm [\Delta\sigma(r_{d(a)}, x)]_{n(p)}$ ,

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

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

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

Therefore, from Equations (6) and (7), one obtains the expressions for relative dielectric constant  $\epsilon(r_{d(a)}, x)$  and energy band gap  $E_{gn(gp)}(r_{d(a)}, x)$ , as:

(i)-for  $r_{d(a)} \geq r_{do(ao)}$ , since  $\epsilon(r_{d(a)}, x) = \frac{\epsilon_0(x)}{\sqrt{1 + \left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3}} \leq \epsilon_0(x)$ , being a **new**

$\epsilon(r_{d(a)}, x)$ -law,

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

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

(ii)-for  $r_{d(a)} \leq r_{do(ao)}$ , since  $\epsilon(r_{d(a)}, x) = \frac{\epsilon_0(x)}{\sqrt{1 - \left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3}} \geq \epsilon_0(x)$ , with a condition,

given by:  $\left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 < 1$ , being a **new**  $\epsilon(r_{d(a)}, x)$ -law,

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

corresponding to the decrease in both  $E_{gn(gp)}(r_{d(a)}, x)$  and  $E_{d(a)}(r_{d(a)}, x)$ , with decreasing  $r_{d(a)}$  and for a given  $x$ ; therefore, the effective Bohr radius  $a_{Bn(Bp)}(r_{d(a)}, x)$  is defined by:

$$a_{Bn(Bp)}(r_{d(a)}, x) \equiv \frac{\epsilon(r_{d(a)}, x) \times \hbar^2}{m_{c(v)}(x) \times q^2} = 0.53 \times 10^{-8} \text{ cm} \times \frac{\epsilon(r_{d(a)}, x)}{m_{c(v)}(x)/m_0}. \quad (8c)$$

Furthermore, it is interesting to remark that the critical total donor (acceptor)-density in the metal-insulator transition (MIT) at  $T=0$  K,  $N_{CDn(NDp)}(r_{d(a)}, x)$ , was given by the Mott's criterium, with an empirical parameter,  $M_{n(p)}$ , as:

$$N_{CDn(CDp)}(r_{d(a)}, x)^{1/3} \times a_{Bn(Bp)}(r_{d(a)}, x) = M_{n(p)}, \quad M_{n(p)} = 0.25, \quad (9a)$$

depending thus on our **new**  $\epsilon(r_{d(a)}, x)$ -law.

This excellent one can be explained from the definition of the reduced effective Wigner-Seitz (WS) radius  $r_{sn(sp)}$ , characteristic of interactions, by:

$$r_{sn(sp)}(N, r_{d(a)}, x) \equiv \left(\frac{3}{4\pi N}\right)^{1/3} \times \frac{1}{a_{Bn(Bp)}(r_{d(a)}, x)} = 1.1723 \times 10^8 \times \left(\frac{1}{N}\right)^{1/3} \times \frac{m_{c(v)}(x)/m_0}{\epsilon(r_{d(a)}, x)}, \quad (9b)$$

being equal to, in particular, at  $N=N_{CDn(CDp)}(r_{d(a)}, x)$ :  $r_{sn(sp)}(N_{CDn(CDp)}(r_{d(a)}, x), r_{d(a)}, x) = 2.4814$ , for any

$(r_{d(a)}, x)$ -values. So, from Eq. (9b), one also has:

$$N_{CDn(CDp)}(r_{d(a)}, x)^{1/3} \times a_{Bn(Bp)}(r_{d(a)}, x) = \left(\frac{3}{4\pi}\right)^{1/3} \times \frac{1}{2.4814} = 0.25 = (WS)_{n(p)} \equiv M_{n(p)}, \quad (9c)$$

being identical to that given in above Eq. (9a).

Thus, the above Equations (9a, 9b, 9c) confirm our new  $\varepsilon(r_{d(a)}, x)$ -law, given in Equations (8a, 8b).

Furthermore, by using  $M_{n(p)} = 0.25$ , according to the empirical Heisenberg parameter  $\mathcal{H}_{n(p)} = 0.47137$ , as those given in Equations (8, 15) of the Ref.<sup>[1]</sup>, we have also showed that  $N_{CDn(CDP)}$  is just the density of electrons (holes) localized in the exponential conduction (valence)-band tail, with a precision of the order of  $2.82 \times 10^{-7}$ . Therefore, the density of electrons (holes) given in parabolic conduction (valence) bands can be defined, as that given in compensated materials, by:

$$N^*(N, r_{d(a)}, x) \equiv N - N_{CDn(CDP)}(r_{d(a)}, x). \tag{9d}$$

**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<sup>[2]</sup>:

$$E_{gin(gip)}(r_{d(a)}, x, T) \text{ in eV} = E_{gn(gp)}(r_{d(a)}, x) - \frac{10^{-4} \times T^2}{T+94K} \times \{7.0043 \times x + 4.3779 \times (1-x)\}, \tag{10}$$

suggesting that, for given x and  $r_{d(a)}$ ,  $E_{gin(gip)}$  decreases with an increasing T, as observed in next Table 1 in Appendix 1.

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

$$n_{in(ip)}^2(r_{d(a)}, x, T) \equiv N_c(T, x) \times N_v(T, x) \times \exp\left(\frac{-E_{gin(gip)}(r_{d(a)}, x, T)}{k_B T}\right), \tag{11}$$

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

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

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

Here, as given in our previous works<sup>[1,2]</sup>, the Fermi energy  $E_{Fn}(-E_{Fp})$ , band gap narrowing (BGN), and apparent band gap narrowing (ABGN), are reported in the following.

First, the reduced Fermi energy  $\eta_{n(p)}$  or the Fermi energy  $E_{Fn}(-E_{Fp})$ , obtained for any T and any effective d(a)-density,  $N^*(N, r_{d(a)}, x) = N^*$ , defined in Eq. (9d), for a simplicity of presentation, being investigated in our previous paper<sup>[8]</sup>, with a precision of the order of  $2.11 \times 10^{-4}$ , is found to be given by:

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

where  $u$  is the reduced electron density,  $u(N^*, T, x) \equiv \frac{N^*}{N_{C(v)}(T, x)}$ ,  
 $F(u) = au^{\frac{2}{3}} \left( 1 + bu^{-\frac{4}{3}} + cu^{-\frac{5}{3}} \right)^{\frac{2}{3}}$ ,  $a = [(3\sqrt{\pi}/4) \times u]^{2/3}$ ,  $b = \frac{1}{9} \left( \frac{\pi}{2} \right)^2$ ,  $c = \frac{62.2739855}{1920} \left( \frac{\pi}{2} \right)^4$ , and  
 $G(u) \simeq \ln(u) + 2^{-\frac{5}{2}} \times u \times e^{-du}$ ;  $d = 2^{3/2} \left[ \frac{1}{\sqrt{27}} - \frac{5}{16} \right] > 0$ .

Here, one notes that: (i) as  $u \gg 1$ , according to the HD [d(a)- X(x)- alloy] 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 LD [a(d)- X(x)- alloy] BR-case, or to the non-degenerate case, Eq. (12) is reduced to the function G(u), noting that the notations: **HD(LD)** and **ER(BR)** denote the heavily doped (lightly doped)-cases and emitter (base)-regions, respectively.

So, the numerical results of  $B_{do(ao)}$ ,  $\epsilon$ ,  $E_{gn(gp)}$ ,  $N_{CDn(CDp)}$ ,  $E_{gin(gp)}(r_{d(a)}, x, T)$ , and  $\eta_{n(p)}(u)$  are calculated, using Equations (5), (8a, 8b), (9a), (10), and (12), respectively, and reported in Table 1 in Appendix 1.

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

$$r_{sn(sp)}(N^*, r_{d(a)}, x) = 1.1723 \times 10^8 \times \left( \frac{1}{N^*} \right)^{1/3} \times \frac{m_{c(v)}(x)}{\epsilon(r_{d(a)}, x)}, \tag{13a}$$

the correlation energy of an effective electron gas,  $E_{cn(cp)}(N^*, r_{d(a)}, x)$ , is given as:

$$E_{cn(cp)}(N^*, r_{d(a)}, x) = \frac{-0.87553}{0.0908 + r_{sn(sp)}} + \frac{0.87553 + \left( \frac{2[1 - \ln(2)]}{\pi^2} \right) \times \ln(r_{sn(sp)}) - 0.093288}{1 + 0.03847728 \times r_{sn(sp)}^{1.67878876}}. \tag{13b}$$

Then, taking into account various spin-polarized chemical potential-energy contributions such as: 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 in the following.

In the n-type HD X(x)- alloy, the BGN is found to be given by<sup>[2]</sup>:

$$\Delta E_{gn}(N^*, r_{d}, x) \simeq a_1 \times \frac{\epsilon_0(x)}{\epsilon(r_{d}, x)} \times N_r^{1/3} + a_2 \times \frac{\epsilon_0(x)}{\epsilon(r_{d}, x)} \times N_r^{\frac{2}{3}} \times (2.503 \times [-E_{cn}(r_{sn}) \times r_{sn}]) + a_3 \times \left[ \frac{\epsilon_0(x)}{\epsilon(r_{d}, x)} \right]^{5/4} \times \sqrt{\frac{m_v}{m_c}} \times N_r^{1/4} + a_4 \times \sqrt{\frac{\epsilon_0(x)}{\epsilon(r_{d}, x)}} \times N_r^{1/2} \times 2 + a_5 \times \left[ \frac{\epsilon_0(x)}{\epsilon(r_{d}, x)} \right]^{\frac{5}{2}} \times N_r^{\frac{2}{3}}, \tag{14n}$$

$$N_r \equiv \left( \frac{N^*}{N_{CDn}(r_{d}, x)} \right),$$

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

$$\Delta E_{gp}(N^*, r_a, x) \simeq a_1 \times \frac{\epsilon_0(x)}{\epsilon(r_a, x)} \times N_r^{1/3} + a_2 \times \frac{\epsilon_0(x)}{\epsilon(r_a, x)} \times N_r^{1/3} \times (2.503 \times [-E_{cp}(r_{sp}) \times r_{sp}]) + a_3 \times \left[ \frac{\epsilon_0(x)}{\epsilon(r_a, x)} \right]^{5/4} \times \sqrt{\frac{m_c}{m_v}} \times N_r^{1/4} + 2a_4 \times \sqrt{\frac{\epsilon_0(x)}{\epsilon(r_a, x)}} \times N_r^{1/2} + a_5 \times \left[ \frac{\epsilon_0(x)}{\epsilon(r_a, x)} \right]^{3/2} \times N_r^{1/6}$$

$$, N_r \equiv \left( \frac{N^*}{N_{CDP}(r_a, x)} \right), \quad (14p)$$

where  $a_1 = 3.15 \times 10^{-3}(\text{eV})$  ,  $a_2 = 5.41 \times 10^{-4}(\text{eV})$  ,  $a_3 = 2.32 \times 10^{-3}(\text{eV})$  ,  
 $a_4 = 4.195 \times 10^{-3}(\text{eV})$  and  $a_5 = 9.80 \times 10^{-5}(\text{eV})$ .

Therefore, in the HD[d(a)-  $X(x)$ - alloy] ER, we can define the effective extrinsic carrier concentration,  $n_{en(ep)}^*$ , by :

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

where the apparent band gap narrowing,  $\Delta E_{agn(agnp)}$ , is found to be defined by:

$$\Delta E_{agn}(N^*, r_{d(a)}, x, T) \equiv \Delta E_{gn}(N^*, r_d, x) + k_B T \times \ln \left( \frac{N^*}{N_c(T, x)} \right) - E_{Fn}(N^*, T, x), \quad (16n)$$

$$\Delta E_{agnp}(N^*, r_{d(a)}, x, T) \equiv \Delta E_{gp}(N^*, r_a, x) + k_B T \times \ln \left( \frac{N^*}{N_v(T, x)} \right) + E_{Fp}(N^*, T, x). \quad (16p)$$

### TOTAL MINORITY-CARRIER SATURATION CURRENT DENSITY

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

$$J_{OI(II)} \equiv J_{Eno(Epo)} + J_{Bpo(Bno)} \quad (17)$$

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[a(d)- $X(x)$ - alloy]BR

Here,  $J_{Bpo(Bno)}$  is determined by<sup>[2]</sup>:

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

where  $n_{ip(in)}^2(r_{a(d)}, x, T)$  is determined Eq. (11),  $D_{e(h)}(N_{a(d)}, r_{a(d)}, x, T)$  is the minority electron (minority hole) diffusion coefficient:

$$D_e(N_a, r_a, x, T) = \frac{k_B T}{e} \times \left[ 850 + \frac{5750}{1 + \left( \frac{N_a}{8 \times 10^{17} \text{ cm}^{-3}} \right)^{1.8}} \right] \times \left( \frac{\varepsilon(r_a, x)}{\varepsilon_0(x)} \right)^2 \text{ (cm}^2 \text{ s}^{-1}), \tag{19a}$$

$$D_h(N_d, r_d, x, T) = \frac{k_B T}{e} \times \left[ 85 + \frac{1165}{1 + \left( \frac{N_d}{4 \times 10^{17} \text{ cm}^{-3}} \right)^{0.44}} \right] \times \left( \frac{\varepsilon(r_d, x)}{\varepsilon_0(x)} \right)^2 \text{ (cm}^2 \text{ s}^{-1}), \tag{19b}$$

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

$$\tau_{eB}(N_a)^{-1} = \frac{1}{10^{-7}} + 3 \times 10^{-13} \times N_a + 1.83 \times 10^{-31} \times N_a^2, \tag{20a}$$

$$\tau_{hB}(N_d)^{-1} = \frac{1}{10^{-7}} + 11.76 \times 10^{-13} \times N_d + 2.78 \times 10^{-31} \times N_d^2. \tag{20b}$$

***J<sub>Eno(Epo)</sub> in the HD[d(a)- X(x)- alloy]ER***

In the non-uniformly and heavily doped emitter region of d(a)- X(x) devices, the effective Gaussian d(a)-density profile or the d(a) (majority-e(h)) density, is defined in such the HD[d(a)- X(x) alloy] ER-width W, as<sup>[21]</sup>:

$$\rho_{d(a)}(y, N^*, W) = N_{d(a)} \times \exp \left\{ - \left( \frac{y}{W} \right)^2 \times \ln \left[ \frac{N^*}{N_{do(ao)}(W)} \right] \right\} \equiv N^* \times \left[ \frac{N^*}{N_{do(ao)}(W)} \right]^{-\left( \frac{y}{W} \right)^2}, \quad 0 \leq y \leq W, \\ N_{do(ao)}(W) \equiv 7.9 \times 10^{17} (2 \times 10^5) \times \exp \left\{ - \left( \frac{W}{184.2 (1) \times 10^{-7} \text{ cm}} \right)^{1.066 (0.5)} \right\} \text{ (cm}^{-3}), \tag{21}$$

where  $\rho_{d(a)}(y = 0) = N^*$  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:

$$N_{d(a)}^{\#}(y, N^*, r_{d(a)}, x, T) \equiv \rho_{d(a)}(y) / \exp \left[ \frac{\Delta E_{agn(agg)}(\rho_{d(a)}, r_{d(a)}, x, T)}{k_B T} \right], \\ N_{d(a)}^{\#}(y = 0, N^*, r_{d(a)}, x, T) \equiv \frac{N^*}{\exp \left[ \frac{\Delta E_{agn(agg)}(N^*, r_{d(a)}, x, T)}{k_B T} \right]}, \text{ and} \\ N_{d(a)}^{\#}(y = W, r_{d(a)}, x, T) \equiv \frac{N_{do(ao)}(W)}{\exp \left[ \frac{\Delta E_{agn(agg)}(N_{do(ao)}(W), r_{d(a)}, x, T)}{k_B T} \right]}, \tag{22}$$

where the apparent band gap narrowing  $\Delta E_{agn(agg)}$  is determined in Equations (16n, 16p), replacing  $N^*$  by  $\rho_{d(a)}(y, N^*, W)$ .

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

$$F_{h(e)}(y, N^*, r_{d(a)}, x, T) \equiv \frac{N^*}{D_{h(e)} \times \exp \left[ \frac{\Delta E_{agn(agg)}}{k_B T} \right]} \text{ (cm}^{-5} \times \text{s)}, \tag{23}$$

being related to the minority hole (electron) diffusion length,  $L_{h(e)}(y, N^*, r_{d(a)}, x, T)$ , as:



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

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

$$\tau_{h(e)} \equiv \frac{1}{D_{h(e)} \times L_{h(e)}^{-2}} = \frac{1}{D_{h(e)} \times (C \times F_{h(e)})^2}. \tag{24}$$

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:

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

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

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

which must verify the two following boundary conditions as:

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

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

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

Further, from the Fick's law for minority hole (electron)-diffusion equations, one has<sup>[1,2]</sup>:

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

where  $N_{d(a)}^{\#}(y, N^*, r_{d(a)}, x, T)$  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:

$$\frac{dJ_{h(e)}(y, N^*, r_{d(a)}, x, T)}{dy} = -e(+e) \times n_i^2 n(p) \times \frac{u(y)}{F_{h(e)}(y) \times L_{h(e)}^2(y)} = -e(+e) \times n_i^2 n(p) \times \frac{u(y)}{N_{d(a)}^{\#}(y, N^*, r_{d(a)}, x, T) \times \tau_{h(e)}}, \tag{28}$$

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

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

Then, taking into account the two above boundary conditions given in Eq. (26), one thus gets the general solution of this Eq. (29), as:

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

where the factor  $I(W, S)$  is determined by:

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

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<sup>4</sup>/s), for the X(x)-alloy, being an empirical parameter, chosen for each crystalline semiconductor, P(y) is thus found to be defined by:

$$P(y) \equiv \int_0^y \frac{dy}{L_{h(e)}(y)}, \quad 0 \leq y \leq W, \quad P(y = W) \equiv \left(\frac{1}{W} \times \int_0^W \frac{dy}{L_{h(e)}(y)}\right) \times W \equiv \frac{W}{L_{h(e)}^{\#}(y)} = \frac{L_{h(e)}(y)}{L_{h(e)}^{\#}(y)} \times \frac{W}{L_{h(e)}(y)}, \quad (32)$$

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:

$$J_{h(e)}(y, W, N^*, r_{d(a)}, x, T, S, V) = -J_{Eno}(y, W, N^*, r_{d(a)}, x, T, S) \left[ J_{Epo}(y, W, N^*, r_{d(a)}, x, T, S) \times \left( \exp\left(\frac{V}{nI(I)(V) \times \tau_T}\right) - 1 \right) \right], \quad (33)$$

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

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

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

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

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

and then,

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

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

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

the effective minority hole (minority electron) transit time [ *htt(ett)* ] by:

$\tau_{h_{eff}}^{\pm}(y = W, W, N^*, r_{d(a)}, x, T, S) \equiv Q_{h(e)}^{\pm}(y = W, W, N^*, r_{d(a)}, x, T) / J_{Eno(Epo)}(y = W, W, N^*, r_{d(a)}, x, T, S)$  , and from Equations (24, 31), one obtains:

$$\frac{\tau_{h_{eff}}^{\pm}(y=W, W, N^*, r_{d(a)}, x, T, S)}{\tau_{hE(eE)}} \equiv 1 - \frac{J_{Eno(Epo)}(y=0, W, N^*, r_{d(a)}, x, T, S)}{J_{Eno(Epo)}(y=W, W, N^*, r_{d(a)}, x, T, S)} = 1 - \frac{1}{\cosh(P) + I \times \sinh(P)} \quad (38)$$

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

As  $P \ll 1$  (or  $W \ll L_{h(e)}$ ) and  $S \rightarrow \infty$ ,  $I \equiv I(W, S) = \frac{D_{h(e)}(N_{do(ao)}(W), r_{d(a)}, x, T)}{S \times L_{h(e)}(N_{do(ao)}(W), r_{d(a)}, x, T)} \rightarrow 0$ , from Eq. (38),

one has:  $\frac{\tau_{h_{eff}}^{\pm}(y=W, W, N^*, r_{d(a)}, x, T, S)}{\tau_{hE(eE)}} \rightarrow 0$  , suggesting a completely transparent emitter region (CTER)-case, where, from Eq. (36), one obtains:

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

Further, as  $P \gg 1$  (or  $W \gg L_{h(e)}$ ) and  $S \rightarrow 0$  ,

$I \equiv I(y = W, r_{d(a)}, x, S) = \frac{D_{h(e)}(N_{do(ao)}(W), r_{d(a)}, x, T)}{S \times L_{h(e)}(N_{do(ao)}(W), r_{d(a)}, x, T)} \rightarrow \infty$  , and from Eq. (38) one has:

$\frac{\tau_{h_{eff}}^{\pm}(y=W, W, N^*, r_{d(a)}, x, T, S)}{\tau_{hE(eE)}} \rightarrow 1$  , suggesting a completely opaque emitter region (COER)-case, where, from Eq. (36), one gets:

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

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:

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

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

$$J_{scI1(scI2)} = J_{scII1(scII2)}$$

### PHOTOVOLTAIC CONVERSION EFFECT AT 300K

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

$$W = 0.1 \mu\text{m}, N = 10^{20} \text{ cm}^{-3}, r_{d(a)}, x, S = 100 \left(\frac{\text{cm}}{\text{s}}\right); N_{a(d)} = 10^{17} \text{ cm}^{-3}, r_{a(d)}, x, \quad (42)$$

we propose, at given open circuit voltages:  $V_{ocI1(ocI2)} = V_{ocII1(ocII2)}$ , the corresponding data of the short circuit current density  $J_{scI1(scI2)} = J_{scII1(scII2)}$  in order to formulate our following treatment method of two fix points, as:

$$\begin{aligned}
 & \text{at } V_{ocI1(ocI2)}(V) = V_{ocII1(ocII2)}(V) = 0.73 \text{ (0.8759)}, \\
 & J_{scI1(scI2)}(\text{mA/cm}^2) = J_{scII1(scII2)}(\text{mA/cm}^2) = 21.6 \text{ (30.25)}. \quad (43)
 \end{aligned}$$

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:

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

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:  $J_{ph.}(V = V_{oc}) \equiv J_{scI(scII)}(W, N^*, T, r_{d(a)}, x, S; N_{a(d)}, T, r_{a(d)}, x, V_{oc})$ , for  $V_{oc} \geq V_{ocI1(ocII1)}$ .

Therefore, the photovoltaic conversion effect occurs, according to:

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

where  $n_{I(II)}(V_{oc}) \equiv n_{I(II)}(W, N^*, r_{d(a)}, x, T, S; N_{a(d)}, r_{a(d)}, x, T; V_{oc})$ , 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  $J_{ol(II)}$  have the same variations, obtained in the same physical conditions, as observed in the following calculation, (ii) the function  $(e^{X_{I(II)}(V_{oc})} - 1)$  or the PVCF,  $n_{I(II)}$ , representing the photovoltaic conversion effect, converts the light, represented by  $J_{scI(scII)}$ , into the electricity, by  $J_{ol(olI)}$ , and finally, for given  $(W, N^*, r_{d(a)}, x, T, S; N_{a(d)}, r_{a(d)}, x, T; V_{oc})$ -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  $n_{I1(II1)}(V_{ocI1(ocII1)})$  and  $n_{I2(II2)}(V_{ocI2(ocII2)})$ , as functions of  $V_{oc}$ , by:

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

where, for example, the values of  $\alpha(\beta)$ , obtained for  $x = (0, 0.5 \text{ and } 1)$ , will be reported in next Tables 3n and 5p in Appendix 1, for these X(x) –alloy junctions.

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

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

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

$$\eta_{I(II)}(W, N^*, r_{d(a)}, x, T, S; N_{a(d)}, r_{a(d)}, x, T; V_{oc}) \equiv \frac{I_{scI(ocII)} \times V_{oc} \times F_{I(II)}}{P_{in}}, \quad (48)$$

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  $\eta_{I(II)}$ ,  $\eta_{I_{max.(II_{max.})}}$ , are obtained at the corresponding ones of  $V_{oc} = V_{ocI(ocII)}$ , at which

$$\left( \frac{\partial \eta_{I(II)}(W, N^*, r_{d(a)}, x, T, S; N_{a(d)}, r_{a(d)}, x, T; V_{oc})}{\partial V_{oc}} \right)_{V_{oc}=V_{ocI(ocII)}} = 0, \text{ as those given in next Tables 3n and 5p}$$

in Appendix 1, being marked in bold. Further, from the well-known Carnot's theorem, being obtained by the second principle in thermodynamics, or 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,  $T_H - T_C$ ,  $T_C \equiv T = 300 \text{ K}$ , to the H-reservoir temperature,  $T_H$ , expressed as:

$$\eta_{I(II)}(T, V_{oc}) \leq \eta_{I_{max.(II_{max.})}}(T, V_{oc} = V_{ocI(ocII)}) \equiv \eta_{Carnot} = \frac{T_H - T_C}{T_H}, \quad (49)$$

for a simplicity, noting that both  $\eta_{I_{max.(II_{max.})}}$  and  $T_H$  depend on  $(W, N^*, r_{d(a)}, x, T, S; N_{a(d)}, r_{a(d)}, x, T; V_{ocI(ocII)})$ -parameters.

### NUMERICAL RESULTS AND CONCLUDING REMARKS

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

*HD (Te; Sn) X(x) alloy ER – LD (In; Cd) X(x) – alloy BR* –case, according to: 2 ( $n^+p$ ) – junctions denoted by:  $(Te^+In, Sn^+Cd)$ , and

*HD (In; Cd) X(x) alloy ER – LD (Te; Sn) X(x) – alloy BR* –case, according to: 2 ( $p^+n$ ) – junctions denoted by:  $(In^+Te, Cd^+Sn)$ .

Now, by using the physical conditions, given in Eq. (42), we can determine various photovoltaic conversion coefficients as follows.

**Firs case: HD [ Te; Sn ] X(x) – Alloy ER – LD [ In; Cd ] X(x) – Alloy BR**

Here, there are the 2 ( $n^+p$ ) –  $X(x)$  junctions, being denoted by:  $(Te^+In, Sn^+Cd)$ .

Then, the numerical results of  $\frac{\tau_{hEt}}{\tau_{hE}}$ ,  $J_{Bpo}$ ,  $J_{Eno}$  and  $J_{oi}$ , are calculated using Equations (38), (18), (36) and (41), respectively, and obtained, as those given in Table 2n in Appendix 1. Further,

those of  $n_I$ ,  $J_{sci}$ ,  $F_I$ ,  $\eta_I$ , and  $T_H$ , are computed, using Equations (46, 45, 47, 48, 49), respectively, and reported in Table 3n in Appendix 1.

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

Here, there are 2 ( $p^+n$ ) – X(x)-junctions, being denoted by: ( $In^+Te, Cd^+Sn$ ).

Then, the numerical results of  $\frac{\tau_{scII}^{\#}}{\tau_{eE}}$ ,  $J_{Bno}$ ,  $J_{Epo}$  and  $J_{oII}$ , are calculated using Equations (38), (18), (36) and (41), respectively, and obtained, as those given in Table 4p in Appendix 1. Further, those of  $n_{II}$ ,  $J_{scII}$ ,  $F_{II}$ ,  $\eta_{II}$ , and  $T_H$ , are computed, using Equations (46, 45, 47, 48, 49), respectively, and reported in Table 5p in Appendix 1.

Finally, some concluding remarks are obtained and discussed as follows.

(1) In Table 3n, for the  $n^+ - p$  X(x) –alloy junction solar cell and for  $r_{Sn(Cd)}$ -radius, one obtains with increasing  $x=(0, 0.5, 1)$ :  $\eta_{II\max.}(\%) = 26.12\%$ ,  $29.91\%$ , **34.18%**, according to  $T_H(\%) = 406.1$  K,  $428.0$  K, **455.8 K**, at  $V_{ocI} = 0.82$  V,  $0.81$  V, **0.80 V**, respectively.

(2) In Table 5p, for the  $p^+ - n$  X(x) –alloy junction solar cell and for  $r_{Cd(Sn)}$ -radius, one obtains with increasing  $x=(0, 0.5, 1)$ :  $\eta_{II\max.}(\%) = 25.03\%$ ,  $29.57\%$ , **33.80%**, according to  $T_H(\%) = 400.2$  K,  $425.9$  K, **453.2 K**, at  $V_{ocII} = 0.82$  V,  $0.81$  V, **0.80 V**, respectively.

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APPENDIX 1

**Table 1.** In the  $[X(x) \equiv CdTe_{1-x}S_x]$ -alloy, in which  $N = 10^{20}cm^{-3}(10^{20}cm^{-3})$  and  $T=300$  K, the numerical results of  $B_{do(a\phi)}$ ,  $\epsilon$ ,  $E_{gn(gp)}$ ,  $N_{CDn(CDP)}$ ,  $E_{gin(gip)}(r_d(a), x, T)$  and  $\eta_{n(p)}$  are computed, using Equations (5), (8a, 8b), (9a), (10) and (12), respectively. Here, on notes that, in the limiting conditions:  $x=(0, 1)$ , these results are reduced to those given in the CdTe- crystal and the CdS -alloy, respectively.

Donor	S		Se	
$r_d$ (nm) ↗	0.104		0.114	
$x$ ↗	0, 0.5, 1		0, 0.5, 1	
$\epsilon(r_d, x)$ ↘	12.942503, 12.1202, 11.298015		11.2257881, 10.51261, 9.799427	
$E_{gno}(r_d, x)$ eV ↗	1.6155583, 2.09222, 2.567913		1.6180978, 2.096666, 2.5748234	
$N_{CDn}(r_d, x)$ in $10^{18} cm^{-3}$ ↗	4.1506041, 18.345022, 55.640067		6.3608576, 28.113996, 85.269163	
$E_{gin}(r_d, x, T)$ in eV ↗	1.51556, 1.96222, 2.40792		1.51809, 1.96667, 2.41483	
$\eta_n \gg 1$ (degenerate case)	32.00, 20.84, 15.44		32.00, 20.83, 15.41	
Donor	Te		Sn	
$r_d$ (nm) ↗	$r_{do}=0.132$		0.140	
$x$ ↗	0, 0.5, 1		0, 0.5, 1	
$B_{do}(x)$ in $10^8$ (N/m <sup>2</sup> ) ↗	2.0211442, 3.541925, 5.5001208			
$\epsilon(r_d, x)$ ↘	10.31, 9.655, 9		10.138688, 9.494571, 8.850455	
$E_{gno}(r_d, x)$ eV ↗	1.62, 2.1, 2.58		1.6204142, 2.100726, 2.5811272	
$N_{CDn}(r_d, x)$ in $10^{18} cm^{-3}$ ↗	8.2108893, 36.290847, 110.06938		8.6341767, 38.161712, 115.74367	
$E_{gin}(r_d, x, T)$ in eV ↗	1.52, 1.97, 2.42		1.52041, 1.9707, 2.42113	
$\eta_n \gg 1$ (degenerate case)	31.999, 20.82, 15.39		31.998, 20.81435, 15.38304	
Acceptor	Ga		Mg	
$r_a$ (nm) ↗	0.126		0.140	
$x$ ↗	0, 0.5, 1		0, 0.5, 1	
$\epsilon(r_a, x)$ ↘	11.41926, 10.69404, 9.9685481		10.444552, 9.781004, 9.1174555	
$E_{gpo}(r_a, x)$ eV ↗	1.6006033, 2.078139, 2.5551356		1.6173143, 2.09697, 2.5765572	
$N_{CDp}(r_a, x)$ in $10^{17} cm^{-3}$ ↗	3.8859101, 4.5690868, 5.4449915		5.0788748, 5.9717851, 7.1165903	
$E_{gip}(r_a, x, T)$ in eV ↗	1.5006, 1.9481, 2.3951		1.5173, 1.967, 2.4166	
$\eta_p \gg 1$ (degenerate case)	6.93, 5.0853, 3.9306		6.9296, 5.0753, 3.9061	
Acceptor	In		Cd	
$r_a$ (nm) ↗	0.144		$r_{ao}=0.148$	
$x$ ↗	0, 0.5, 1		0, 0.5, 1	
$B_{ao}(x)$ in $10^8$ (N/m <sup>2</sup> ) ↗			1.2377251, 1.3950062, 1.5866282	
$\epsilon(r_a, x)$ ↘	10.343599, 9.686465, 9.0293303		10.31, 9.655, 9	
$E_{gpo}(r_a, x)$ eV ↗	1.6193195, 2.099233, 2.5791277		1.62, 2.1, 2.58	
$N_{CDp}(r_a, x)$ in $10^{17} cm^{-3}$ ↗	5.2290386, 6.148349, 7.3270019		5.2803284, 6.208656, 7.398870	
$E_{gip}(r_a, x, T)$ in eV ↗	1.5193, 1.9692, 2.4191		1.52, 1.97, 2.42	
$\eta_p \gg 1$ (degenerate case)	6.9275, 5.0704, 3.894		6.925, 5.0643, 3.879	



**Table 2n.** In the HD [(Te; Sn)-X(x)-alloy] ER-LD[(In; Cd)-X(x)-alloy] BR, for physical conditions given in Eq. (42) and for a given x, our numerical results of  $\frac{\tau_{HE}^+}{\tau_{HE}^-}$ ,  $J_{Bpo}$ ,  $J_{Eno}$  and  $J_{ol}$ , are computed, using Equations (38), (18), (36) and (41), respectively.

$n^+p$	$Te^+In$	$Sn^+Cd$
Here, x=0 for the $(Te^+In, Sn^+Cd)$ -junctions, and from Eq. (38), one obtains: $\frac{\tau_{HE}^+}{\tau_{HE}^-} = (0, 0)$ suggesting a completely transparent condition.		
$J_{Bpo}$ in $10^{-20}$ (A/cm <sup>2</sup> ) ↗	2.5881	2.5965
$J_{Eno}$ in $10^{-25}$ (A/cm <sup>2</sup> ) ↘	6.0916	4.6241
$J_{ol}$ in $10^{-20}$ (A/cm <sup>2</sup> ) ↗	2.5882	2.5966
Here, x=0.5 for the $(Te^+In, Sn^+Cd)$ -junctions, and from Eq. (38), one obtains: $\frac{\tau_{HE}^+}{\tau_{HE}^-} = (0, 0)$ suggesting a completely transparent condition.		
$J_{Bpo}$ in $10^{-27}$ (A/cm <sup>2</sup> ) ↗	1.3215	1.3258
$J_{Eno}$ in $10^{-32}$ (A/cm <sup>2</sup> ) ↘	8.0807	6.8868
$J_{ol}$ in $10^{-27}$ (A/cm <sup>2</sup> ) ↗	1.3216	1.3258
Here, x=1 for the $(Te^+In, Sn^+Cd)$ -junctions, and from Eq. (38), one obtains: $\frac{\tau_{HE}^+}{\tau_{HE}^-} = (0, 0)$ suggesting a completely transparent condition.		
$J_{Bpo}$ in $10^{-35}$ (A/cm <sup>2</sup> ) ↗	5.5307	5.5486
$J_{Eno}$ in $10^{-39}$ (A/cm <sup>2</sup> ) ↘	9.0568	8.0527
$J_{ol}$ in $10^{-35}$ (A/cm <sup>2</sup> ) ↗	5.5316	5.5494

**Table 3n.** In the HD [(Te; Sn)-X(x)-alloy] ER-LD[(In; Cd)-X(x)-alloy] BR, for physical conditions given in Eq. (42) and for a given x, our numerical results of  $n_I$ ,  $J_{scl}$ ,  $F_I$ ,  $\eta_I$ , and  $T_H$ , are computed, using Equations (46, 45, 47, 48, 49), respectively, noting that both  $\eta_{I_{max}}$ , and  $T_H$ , marked in bold, increase with increasing x for given  $r_{d(\alpha)}$ , being new results.

$V_{oc}(V)$	$n_I$	$J_{scl} (\frac{mA}{cm^2})$	$F_I (\%)$	$\eta_I (\%)$
Here, x=0. For the $(Te^+In, Sn^+Cd)$ junctions, the value of $\alpha$ given in Eq. (46) is <b>1.13905</b> .				
$n^+p$	$Te^+In; Sn^+Cd$	$Te^+In; Sn^+Cd$	$Te^+In; Sn^+Cd$	$Te^+In; Sn^+Cd$
<b>0.73</b>	0.684; 0.684	21.6; 21.6	88.79; 88.79	14.00; 14.00
0.81	0.750; 0.750	36.16; 36.16	88.90; 88.90	26.04; 26.03
<b>0.82</b>	0.759; 0.759	35.83; 35.83	88.90; 88.89	<b>26.12; 26.12</b>
			<b><math>V_{ocI} = 0.82 V</math></b>	<b><math>406.1; 406.1 = T_H(K)</math></b>
0.83	0.769; 0.769	35.23; 35.23	88.89; 88.89	26.00; 25.99
<b>0.8759</b>	0.814; 0.814	30.25; 30.25	88.86; 88.86	23.54; 23.54
1	0.946; 0.946	14.45; 14.45	88.71; 88.71	12.82; 12.82

Here,  $x=0.5$ . For the ( $Te^{+}In, Sn^{+}Cd$ ) junctions, the value of  $\alpha$  given in Eq. (46) is **1.13143**.

$n^{+}p$	$Te^{+}In, Sn^{+}Cd$	$Te^{+}In, Sn^{+}Cd$	$Te^{+}In, Sn^{+}Cd$	$Te^{+}In, Sn^{+}Cd$
<b>0.73</b>	0.486; 0.486	21.6; 21.6	91.41; 91.41	14.41; 14.41
0.80	0.527; 0.527	40.71; 40.71	91.48; 91.48	29.79; 29.79
<b>0.81</b>	0.534; 0.534	40.37; 40.37	91.48; 91.48	<b>29.91; 29.91</b>
			<b><math>V_{ocI} = 0.81 V</math></b>	<b><math>428.0; 428.0 = T_H(K)</math></b>
0.82	0.541; 0.541	39.56; 39.56	91.48; 91.48	29.67; 29.67
<b>0.8759</b>	0.580; 0.580	30.24; 30.24	91.45; 91.45	24.22; 24.22
1	0.675; 0.675	10.47; 10.47	91.32; 91.32	9.565; 9.565

Here,  $x=1$ . For the ( $Te^{+}In, Sn^{+}Cd$ ) junctions, the value of  $\alpha$  given in Eq. (46) is **1.1273**.

$n^{+}p$	$Te^{+}In, Sn^{+}Cd$	$Te^{+}In, Sn^{+}Cd$	$Te^{+}In, Sn^{+}Cd$	$Te^{+}In, Sn^{+}Cd$
<b>0.73</b>	0.376; 0.376	21.6; 21.6	92.99; 92.99	14.66; 14.66
0.79	0.403; 0.403	45.90; 45.90	93.05; 93.05	33.74; 33.74
<b>0.80</b>	0.408; 0.408	45.92; 45.92	93.05; 93.05	<b>34.18; 34.18</b>
			<b><math>V_{ocI} = 0.80 V</math></b>	<b><math>455.8; 455.8 = T_H(K)</math></b>
0.81	0.413; 0.413	45.16; 45.16	93.05; 93.05	34.04; 34.03
<b>0.8759</b>	0.449; 0.449	30.27; 30.27	93.02; 93.02	24.66; 24.66
1	0.523; 0.523	7.575; 7.576	92.91; 92.91	7.039; 7.039

**Table 4p.** In the HD [(In: Cd)-X(x)-alloy] ER-LD[(Te: Sn)-X(x)-alloy] BR, for physical conditions given in Eq. (42) and for a given x, our numerical results of  $\frac{\tau_{sc}^*}{\tau_{se}}$ ,  $J_{Bno}$ ,  $J_{Epo}$  and  $J_{oII}$ , are computed, using Equations (38), (18), (36) and (41), respectively.

$p^{+}n$	$In^{+}Te$	$Cd^{+}Sn$
Here, $x=0$ , and for the ( $In^{+}Te, Cd^{+}Sn$ )-junctions and from Eq. (34), one obtains: $\frac{\tau_{sc}^*}{\tau_{se}} = (0,0)$ suggesting a completely transparent condition.		
$J_{Bno}$ in $10^{-21} (A/cm^2) \searrow$	9.5501	9.2422
$J_{Epo}$ in $10^{-18} (A/cm^2) \searrow$	5.2659	4.4143
$J_{oII}$ in $10^{-18} (A/cm^2) \searrow$	5.2754	4.4226
Here, $x=0.5$ , and for the ( $In^{+}Te, Cd^{+}Sn$ )-junctions and from Eq. (34), one obtains: $\frac{\tau_{sc}^*}{\tau_{se}} = (0,0)$ suggesting a completely transparent condition.		

$J_{Eno}$ in $10^{-28}$ (A/cm <sup>2</sup> ) ↘	4.9354	4.7190
$J_{Epo}$ in $10^{-26}$ (A/cm <sup>2</sup> ) ↘	1.5624	1.2916
$J_{oII}$ in $10^{-26}$ (A/cm <sup>2</sup> ) ↘	1.6118	1.3388

Here,  $x=1$ , and for the  $(In^{+}Te, Cd^{+}Sn)$  junctions and from Eq. (34), one obtains:  $\frac{\tau_{sE}^{+}}{\tau_{sE}} = (0,0)$  suggesting a completely transparent condition.

$J_{Eno}$ in $10^{-35}$ (A/cm <sup>2</sup> ) ↘	2.0979	1.9750
$J_{Epo}$ in $10^{-34}$ (A/cm <sup>2</sup> ) ↘	1.0483	0.9044
$J_{oII}$ in $10^{-34}$ (A/cm <sup>2</sup> ) ↘	1.2581	1.1019

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

$V_{oc}(V)$	$n_{II}$	$J_{scII}(\frac{mA}{cm^2})$	$F_{II}(\%)$	$\eta_{II}(\%)$
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Here,  $x=0$ . For the  $(In^{+}Te, Cd^{+}Sn)$ -junctions, the value of  $\beta$  given in Eq. (46) is **1.143**.

$p^{+}n$	$In^{+}Te; Cd^{+}Sn$	$In^{+}Te; Cd^{+}Sn$	$In^{+}Te; Cd^{+}Sn$	$In^{+}Te; Cd^{+}Sn$
<b>0.73</b>	0.785; 0.782	21.6; 21.6	87.54; 87.59	13.80; 13.81
0.81	0.860; 0.856	34.92; 34.99	87.67; 87.71	24.80; 24.86
<b>0.82</b>	0.871; 0.866	34.73; 34.80	87.67; 87.71	<b>24.96; 25.03</b>
			<b><math>V_{ocI} = 0.82 V</math></b>	<b><math>399.8; 400.2 = T_H(K)</math></b>
0.83	0.882; 0.877	34.30; 34.37	87.66; 87.71	24.95; 25.02
<b>0.8759</b>	0.934; 0.929	30.25; 30.30	87.63; 87.68	23.22; 23.27
1	1.085; 1.080	16.01; 15.98	87.46; 87.51	14.00; 13.98

Here,  $x=0.5$ . For the  $(In^{+}Te, Cd^{+}Sn)$ -junctions, the value of  $\beta$  given in Eq. (46) is **1.1328**.

$p^{+}n$	$In^{+}Te; Cd^{+}Sn$	$In^{+}Te; Cd^{+}Sn$	$In^{+}Te; Cd^{+}Sn$	$In^{+}Te; Cd^{+}Sn$
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0.73	0.508; 0.506	21.6; 21.6	91.10; 91.13	14.36; 14.37
0.80	0.551; 0.549	40.21; 40.30	91.18; 91.21	29.34; 29.40
0.81	0.558; 0.556	39.94; 40.02	91.18; 91.20	29.50; 29.57
			$V_{ocI} = 0.81 V$	$425.5; 425.9 = T_H(K)$
0.82	0.565; 0.563	39.22; 39.30	91.18; 91.20	29.33; 29.39
0.8759	0.606; 0.604	30.47; 30.50	91.15; 91.17	24.33; 24.36
1	0.705; 0.702	11.08; 11.05	91.02; 91.04	10.08; 10.06

Here,  $x=1$ . For the  $(In^+Te, Cd^+Sn)$ -junctions, the value of  $\beta$  given in Eq. (46) is **1.127**.

$p^+n$	$In^+Te, Cd^+Sn$	$In^+Te, Cd^+Sn$	$In^+Te, Cd^+Sn$	$In^+Te, Cd^+Sn$
0.73	0.380; 0.380	21.6; 21.6	92.93; 92.94	14.65; 14.65
0.79	0.408; 0.407	45.37; 45.43	92.99; 92.99	33.33; 33.37
0.80	0.413; 0.412	45.37; 45.43	92.99; 92.99	33.75; 33.80
			$V_{ocI} = 0.80 V$	$452.8; 453.2 = T_H(K)$
0.81	0.418; 0.417	44.61; 44.67	92.99; 92.99	33.60; 33.65
0.8759	0.454; 0.454	30.00; 30.01	92.96; 92.97	24.42; 24.44
1	0.528; 0.528	7.624; 7.608	92.85; 92.86	7.079; 7.065