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OPTICAL COEFFICIENTS IN THE N(P)-TYPE DEGENERATE CdS(1-x) Te(x)-CRYSTALLINE ALLOY, DUE TO THE NEW STATIC DIELECTRIC CONSTANT-LAW AND THE GENERALIZED MOTT CRITERIUM IN THE METAL-INSULATOR TRANSITION. (4)

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ABTRACT

In the n(p)-type $CdS_{1-x}Te_x$- crystalline alloy, with $0 \leq x \leq 1$, basing on our two recent works[1,2], for a given x, and with an increasing $r_{d(a)}$, the optical coefficients have been determined, as functions of the photon energy E, total impurity density N, the donor (acceptor) radius $r_{d(a)}$, concentration x, and temperature T. Those results have been affected by **(i)** the important new $\varepsilon(r_{d(a)}, x)$ -law, developed in Equations (8a, 8b), stating that, for a given x, due to the impurity-size effect, ε decreases (↘) with an increasing (↗) $r_{d(a)}$, and then by **(ii)** the generalized Mott critical d(a)-density defined in the metal-insulator transition (MIT), $N_{CDn(NDp)}(r_{d(a)}, x)$, as observed in Equations (8c, 9a). Furthermore, we also showed that $N_{CDn(NDp)}$ is just the density of carriers localized in exponential band tails, with a precision of the order of 2.84×10^{-7}, as that given in Table 4 of Ref.[1], according to a definition of the effective density of electrons (holes) given in parabolic conduction (valence) bands by: $N^*(N, r_{d(a)}, x) \equiv N - N_{CDn(NDp)}(r_{d(a)}, x)$, as defined in Eq. (9d). In summary, due to the new $\varepsilon(r_{d(a)}, x)$-law and to the effective density of electrons (holes) given in parabolic conduction (valence) bands $N^*(N, r_{d(a)}, x)$, for a given x, and with an increasing $r_{d(a)}$, the numerical

results of all the optical coefficients, obtained in appropriated physical conditions (E, N, T), and calculated by using Equations (15, 16, 20, 21), are reported in Tables 1, 2, 3n, 3p, 4n, 4p, 5n, and 5p in Appendix 1.

KEYWORS: $CdS_{1-x}Te_x$ - crystalline alloy; impurity-size effect; Mott critical impurity density in the MIT, optical coefficients.

INTRODUCTION

Here, basing on our two recent works[1, 2] and also other ones[3-8], all the optical coefficients given in the n(p)-type $\mathbf{X(x) \equiv CdS_{1-x}Te_x}$ - crystalline alloy, with $0 \le x \le 1$, are investigated, as functions of the photon energy E, total impurity density N, the donor (acceptor) radius $r_{d(a)}$, concentration x, and temperature T.

Then, for a given x, and with an increasing $r_{d(a)}$, the numerical results of all the optical coefficients, obtained in appropriated physical conditions (E, N, T), and calculated by using Equations (15, 16, 20, 21), are reported in Tables 1, 2, 3n, 3p, 4n, 4p, 5n, and 5p in Appendix 1.

ENERGY BAND STUCTURE PARAMETERS

First of all, in the $n^+(p^+) - p(n)$ $\mathbf{X(x) \equiv CdS_{1-x}Te_x}$- crystalline alloy at T=0 K, we denote the donor (acceptor) d(a)-radius by $r_{d(a)}$, and also the intrinsic one by: $r_{do(ao)}$=$r_{S(Cd)}$=0.104 nm (0.148 nm).

A. Effect of x- concentration

Here, the intrinsic energy-band-structure parameters [1], 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.

$m_{c(v)}(x)/m_o = 0.095(0.82) \times x + 0.197\ (0.801) \times (1-x)$

(1)

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

$\varepsilon_o(x) = 10.31 \times x + 9 \times (1-x).$

(2)

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

$E_{go}(x) = 1.62 \times x + 2.58 \times (1-x)$.

(3)

Therefore, we can define the effective donor (acceptor)-ionization energy in absolute values as.

$$E_{do(ao)}(x) = \frac{13600 \times [m_{c(v)}(x)/m_o]}{[\varepsilon_o(x)]^2}\ \mathrm{meV}, \quad (4)$$

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. Effect of Impurity $r_{d(a)}$-size, with a given x

Here, the changes in all the energy-band-structure parameters, expressed in terms of the effective relative dielectric constant $\varepsilon(r_{d(a)}, x)$, developed 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, $p_o = 0$, and for the deformation potential energy (or the strain energy) σ, $\sigma_o = 0$. Further, the two important equations[1, 7], 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: $\frac{d}{dV}\left(\frac{d\sigma}{dV}\right) = \frac{B}{V}$. Then, by an integration, one gets.

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

(6)

Furthermore, we also showed 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: $\pm [\Delta\sigma(r_{d(a)}, x)]_{n(p)}$,

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

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

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

(7)

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

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

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

(8a)

according to the increase in both $E_{gn(gp)}\left(r_{d(a)},x\right)$ and $E_{d(a)}\left(r_{d(a)},x\right)$, with increasing $r_{d(a)}$ and 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: $\left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 < 1$, being a **new** $\boldsymbol{\varepsilon(r_{d(a)},x)}$**-law**,

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

(8b)

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

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

(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.

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

(9a)

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

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

(9b)

being equal to, in particular, at N=$N_{CDn(CDp)}(r_{d(a)}, x)$: $r_{sn(sp)}\left(N_{CDn(CDp)}(r_{d(a)}, x), r_{d(a)}, x\right)$= **2.4814**, for any $(r_{d(a)}, x)$-values. So, from Eq. (9b), one also has.

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

(9c)

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

Furthermore, by using $\mathbf{M_{n(p)}} = \mathbf{0.25}$, according to the empirical Heisenberg parameter $\boldsymbol{\mathcal{H}_{n(p)}} = \mathbf{0.47137}$, as those given in Equations (8, 15) of the Ref.[1], 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 $\mathbf{2.84 \times 10^{-7}}$. Therefore, the density of electrons (holes) given in parabolic conduction (valence) bands can be defined, as that given in compensated materials, by.

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

(9d)

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

Here, the intrinsic band gap $E_{gni(gpi)}(r_{d(a)}, x, T)$ at any T is given by:

$E_{gni(gpi)}(r_{d(a)}, x, T) \text{ in eV} = E_{gno(gpo)}(r_{d(a)}, x) - 10^{-4} \times T^{2} \times \left\{\frac{4.3779 \times x}{T+94\,K} + \frac{7.0043 \times (1-x)}{T+94\,K}\right\},$

(10)

suggesting that, for given x and $r_{d(a)}$, $E_{gni(gpi)}$ decreases with an increasing T.

Then, in the following, for the study of optical phenomena, one denote the conduction (valence)-band density of states by $N_{c(v)}(T,x)$ as.

$N_{c(v)}(T,x) = 2 \times g_{c(v)}(x) \times \left(\frac{m_r(x) \times k_B T}{2\pi\hbar^2}\right)^{\frac{3}{2}}$ (cm^{-3}), $g_v(x) \equiv 1 \times x + 1 \times (1-x) = 1$, (11)

where $m_r(x)/m_o$ is the reduced effective mass $m_r(x)/m_o$, defined by.
$m_r(x) \equiv [m_c(x) \times m_v(x)]/[m_c(x) + m_v(x)]$.

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

Here, as given in our previous works[1,2], the Fermi energy $E_{Fn}(-E_{Fp})$, and the band gap narrowing 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[8], with a precision of the order of 2.11×10^{-4}, is found to be given by.

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

where u is the reduced electron density, $u(N, r_{d(a)}, x, T) \equiv \frac{N^*}{N_{c(v)}(T,x)}$,

$F(u) = au^{\frac{2}{3}}\left(1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}}\right)^{-\frac{2}{3}}$, $a = \left[(3\sqrt{\pi}/4) \times u\right]^{2/3}$, $b = \frac{1}{8}\left(\frac{\pi}{a}\right)^2$, $c = \frac{62.3739855}{1920}\left(\frac{\pi}{a}\right)^4$, and $G(u) \simeq Ln(u) + 2^{-\frac{3}{2}} \times u \times e^{-du}$; $d = 2^{3/2}\left[\frac{1}{\sqrt{27}} - \frac{3}{16}\right] > 0$. Therefore, from Eq. (12), the Fermi energies are expressed as functions of variables : $N, r_{d(a)}, x$, and T.

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 in particular at T=0 and as $N^* = 0$, according to the metal-insulator transition (**MIT**), one has: $+E_{Fn}(-E_{Fp}) = \frac{\hbar^2}{2 \times m_r(x)} \times (3\pi^2 N^*)^{2/3} = 0$, 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.

Now, in Eq. (9b), in which one replaces $m_{c(v)}(x)$ by $m_r(x)$, the effective Wigner-Seitz radius becomes as.

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

(13a)

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

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

(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 narrowings are given in the following.

In the n-type HD X(x)- alloy, the BGN is found to be given by.

$$\Delta E_{gn}(N, r_d, x) \simeq a_1 \times \frac{\varepsilon_o(x)}{\varepsilon(r_d, x)} \times N_r^{1/3} + a_2 \times \frac{\varepsilon_o(x)}{\varepsilon(r_d, x)} \times N_r^{\frac{1}{3}} \times (2.503 \times [-E_{cn}(r_{sn}) \times r_{sn}]) + a_3 \times \left[\frac{\varepsilon_o(x)}{\varepsilon(r_d, x)}\right]^{5/4} \times \sqrt{\frac{m_v}{m_r}} \times N_r^{1/4} + a_4 \times \sqrt{\frac{\varepsilon_o(x)}{\varepsilon(r_d, x)}} \times N_r^{1/2} \times 2 + a_5 \times \left[\frac{\varepsilon_o(x)}{\varepsilon(r_d, x)}\right]^{\frac{3}{2}} \times N_r^{\frac{1}{6}}, \quad N_r \equiv \left(\frac{N^*}{N_{CDn}(r_d, x)}\right),$$

(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.

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

(14p)

where $a_1 = 3.15 \times 10^{-3}(\mathrm{eV})$, $a_2 = 5.41 \times 10^{-4}(\mathrm{eV})$, $a_3 = 2.32 \times 10^{-3}(\mathrm{eV})$, $a_4 = 4.12 \times 10^{-3}(\mathrm{eV})$ and $a_5 = 9.8 \times 10^{-5}(\mathrm{eV})$.

One also remarks that, as $N^* = 0$, according to the MIT, $\Delta E_{gn(gp)}(N, r_{d(a)}, x) = 0$.

OPTICAL BAND GAP

Here, the optical band gap is found to be defined by:

$$E_{gn1(gp1)}(N, r_{d(a)}, x, T) \equiv E_{gni(gpi)}(r_{d(a)}, x, T) - \Delta E_{gn(gp)}(N, r_{d(a)}, x) + (-)E_{Fn(Fp)}(N, r_{d(a)}, x, T), \quad (15)$$

where $E_{gin(gip)}$, $[+E_{Fn}, -E_{Fp}] \geq 0$, and $\Delta E_{gn(gp)}$ are respectively determined in Equations [10, 12, 14n(p)], respectively. So, as noted above, at the MIT, Eq. (15) thus becomes: $E_{gn1(gp1)}(r_{d(a)}, x) = E_{gno(gpo)}(r_{d(a)}, x)$, according to: $N = N_{CDn(NDp)}(r_{d(a)}, x)$.

OPTICAL COEFFICIENTS

The optical properties of any medium can be described by the complex refraction index $\mathbb{N}$ and the complex dielectric function ε, $\mathbb{N} \equiv n - i\kappa$ and $\varepsilon \equiv \varepsilon_1 - i\varepsilon_2$, where $i^2 = -1$ and $\varepsilon \equiv \mathbb{N}^2$. Therefore, the real and imaginary parts of ε denoted by ε_1 and ε_2 can thus be expressed in terms of the refraction index n and the extinction coefficient κ as: $\varepsilon_1 \equiv n^2 - \kappa^2$ and $\varepsilon_2 \equiv 2n\kappa$. One notes that the optical absorption coefficient α is related to ε_2, n, κ, and the optical conductivity σ_O, by[2]

$$\alpha(E, N, r_{d(a)}, x, T) \equiv \frac{\hbar q^2 \times |v(E)|^2}{n(E) \times \varepsilon_{\text{free space}} \times cE} \times J(E^*) = \frac{E \times \varepsilon_2(E)}{\hbar c n(E)} \equiv \frac{2E \times \kappa(E)}{\hbar c} \equiv \frac{4\pi\sigma_O(E)}{cn(E) \times \varepsilon_{\text{free space}}}, \ \varepsilon_1 \equiv n^2 - \kappa^2 \text{ and } \varepsilon_2 \equiv 2n\kappa, \quad (16)$$

where, since $E \equiv \hbar\omega$ is the photon energy, the effective photon energy: $\mathbf{E^* = E - E_{gn1(gp1)}(N, r_{d(a)}, x, T)}$ is thus defined as the reduced photon energy.

Here, -q, $\hbar$, $|v(E)|$, ω, $\varepsilon_{\text{free space}}$, c and $J(E^*)$ respectively represent: the electron charge, Dirac's constant, matrix elements of the velocity operator between valence (conduction)-and-conduction (valence) bands in n(p)-type semiconductors, photon frequency, permittivity of free space, velocity of light, and joint density of states. It should be noted that, if the three functions such as: $|v(E)|^2$, $J(E^*)$ and $n(E)$ are known, then the other optical dispersion functions as those given in Eq. (16) can thus be determined. Moreover, the normal-incidence reflectance, $R(E)$, can be expressed in terms of $\kappa(E)$ and $n(E)$ as.

$R(E, N, r_{d(a)}, x, T) = \frac{[n(E)-1]^2+\kappa(E)^2}{[n(E)+1]^2+\kappa(E)^2}$.

(17)

From Equations (16, 17), if the two optical functions, ε_1 and ε_2, (or n and κ), are both known, the other ones defined above can thus be determined, noting also that: $\mathbf{E_{gn1(gp1)}(N, r_{d(a)}, x, T) = E_{gn1(gp1)}}$, for a presentation simplicity.

Then, one has

-at low values of $E \gtrsim E_{gn1(gp1)}$,

$J_{n(p)}(E, N, r_{d(a)}, x, T) = \frac{1}{2\pi^2} \times \left(\frac{2m_r}{\hbar^2}\right)^{3/2} \times \frac{(E-E_{gn1(gp1)})^{a-(1/2)}}{E_{gni(gpi)}^{a-1}} = \frac{1}{2\pi^2} \times \left(\frac{2m_r}{\hbar^2}\right)^{3/2} \times (E - E_{gn1(gp1)})^{1/2}$, for a=1,

(18)

and at large values of $E > E_{gn1(gp1)}$,

$J_{n(p)}(E, N, r_{d(a)}, x, T) = \frac{1}{2\pi^2} \times \left(\frac{2m_r}{\hbar^2}\right)^{3/2} \times \frac{(E-E_{gn1(gp1)})^{a-(1/2)}}{E_{gni(gpi)}^{a-1}} = \frac{1}{2\pi^2} \times \left(\frac{2m_r}{\hbar^2}\right)^{3/2} \times \frac{(E-E_{gn1(gp1)})^{2}}{E_{gni(gpi)}^{3/2}}$, for

a=5/2. (19)

Further, one notes that, as $E \to \infty$, Forouhi and Bloomer (FB) [4] claimed that $\kappa(E \to \infty) \to$ a constant, while the $\kappa(E)$ -expressions, proposed by Van Cong [2] quickly go to 0 as E^{-3}, and consequently, their numerical results of the optical functions such as: $\sigma_O(E)$ and $\alpha(E)$, given in Eq. (16), both go to 0 as E^{-2}.

Now, an improved Forouhi-Bloomer parameterization model (FB-PM), used to determine the expressions of the optical coefficients in the degenerate $n^+(p^+) - p(n)\, X(x)$- crystalline alloy, is now proposed as follows. Then, if denoting the functions G(E) and F(E) and by: $G(E) \equiv \sum_{i=1}^{4} \frac{A_i}{E^2 - B_i E + C_i}$ and $F(E) \equiv \sum_{i=1}^{4} \frac{A_i}{E^2 \times (1+10^{-4} \times \frac{E}{6}) - B_i E + C_i}$, we propose.

$\kappa(E, N, r_{d(a)}, x, T) = G(E) \times E_{gni(gpi)}^{3/2} \times \left(E^* \equiv E - E_{gn1(gp1)}\right)^{1/2}$, for $E_{gni(gpi)} \leq E \leq 2.3$ eV,

$= F(E) \times \left(E^* \equiv E - E_{gn1(gp1)}\right)^2$, for $E \geq 2.3$ eV ,

(20)

being equal to 0 for $E^* = 0$ (or for $E = E_{gn1(gp1)}$), and also going to 0 as E^{-1} as $E \to \infty$, and further,

$$n(E, N, r_{d(a)}, x, T) = n_{\infty}(r_{d(a)}, x) + \sum_{i=1}^{4} \frac{X_i(E_{gn1(gp1)}) \times E + Y_i(E_{gn1(gp1)})}{E^2 - B_i E + C_i} \quad .$$

(21)

going to a constant as $E \to \infty$, since $n(E \to \infty, r_{d(a)}, x) \to n_{\infty}(r_{d(a)}, x) = \sqrt{\varepsilon(r_{d(a)}, x)} \times \frac{\omega_T}{\omega_L}$, $\omega_T = 5.1 \times 10^{13}\ s^{-1}$ [5] and $\omega_L = 8.9755 \times 10^{13}\ s^{-1}$.

Here, the other parameters are determined by:

$X_i(E_{gn1(gp1)}) = \frac{A_i}{Q_i} \times \left[-\frac{B_i^2}{2} + E_{gn1(gp1)} B_i - E_{gn1(gp1)}^2 + C_i\right]$,

$Y_i(E_{gn1(gp1)}) = \frac{A_i}{Q_i} \times \left[\frac{B_i \times (E_{gn1(gp1)}^2 + C_i)}{2} - 2E_{gn1(gp1)} C_i\right]$, $Q_i = \frac{\sqrt{4C_i - B_i^2}}{2}$, where, for i=(1, 2, 3, and 4), $A_i = 1.154 \times A_{i(FB)} = 4.7314 \times 10^{-4},\ 0.2314, 0.1118$ and 0.0116, $B_i \equiv B_{i(FB)} = 5.871, 6.154, 9.679$ and 13.232, and $C_i \equiv C_{i(FB)} = 8.619, 9.784, 23.803$, and 44.119.

Then, as noted above, if the two optical functions, n and κ, are both known, the other ones defined in Equations (16, 17) can also be determined.

NUMERICAL RESULTS

Now, some numerical results of those optical functions are investigated in the n(p)-type $\mathbf{X(x) \equiv CdS_{1-x}Te_x}$- crystalline alloy, as follows.

A. Metal-insulator transition (MIT)-case

As discussed above, the physical conditions used for the MIT are found to be given by: T=0K, $N^* = 0$ or $N = N_{CDn(CDp)}$, giving rise to:

$E_{gn1(gp1)}(N^* = 0, r_{d(a)}, x, T = 0) = E_{gn1(gp1)}(r_{d(a)}, x) = E_{gno(gpo)}(r_{d(a)}, x)$.

Then, in this MIT-case, if $E = E_{gn1(gp1)}(r_{d(a)}, x) = E_{gno(gpo)}(r_{d(a)}, x)$, which can be defined as the **critical photon energy**: $E \equiv E_{CPE}(r_{d(a)}, x)$, one obtains: $\kappa_{MIT}(r_{d(a)}, x) = 0$ from Eq. (20), and from Eq. (16): $\varepsilon_{2(MIT)}(r_{d(a)}, x) = 0$, $\sigma_{O(MIT)}(r_{d(a)}, x) = 0$ and $\propto_{MIT}(r_{d(a)}, x) = 0$, and the other functions such as : $n_{MIT}(r_{d(a)}, x)$ from Eq. (21), and $\varepsilon_{1(MIT)}(r_{d(a)}, x)$ and $R_{MIT}(r_{d(a)}, x)$ from Eq. (16) decrease with increasing $r_{d(a)}$ and E_{CPE}, as those investigated in Table 1 in Appendix 1.

B. Optical coefficients, obtained as E → ∞

In Eq. (21), at any T, the choice of the real refraction index: $n(E \to \infty, r_{d(a)}, x, T) = n_{\infty}(r_{d(a)}, x) = \sqrt{\varepsilon(r_{d(a)}, x)} \times \frac{\omega_T}{\omega_L}$, $\omega_T = 5.1 \times 10^{13}\ s^{-1}$ [5] and $\omega_L = 8.9755 \times 10^{13}\ s^{-1}$, was obtained from the Lyddane-Sachs-Teller relation[5], from which T(L) represent the transverse (longitudinal) optical phonon modes. Then, from Equations (16, 17, 20), from such the asymptotic behavior ($E \to \infty$), we obtain: $\kappa_{\infty}(r_{d(a)}, x) \to 0$ and $\varepsilon_{2,\infty}(r_{d(a)}, x) \to 0$, as E^{-1}, so that $\varepsilon_{1,\infty}(r_{d(a)}, x)$, $\sigma_{O,\infty}(r_{d(a)}, x)$, $\alpha_{\infty}(r_{d(a)}, x)$ and $R_{\infty}(r_{d(a)}, x)$ go to their appropriate limiting constants, as those investigated in Table 2 in Appendix 1.

C. Variations of some optical coefficients, obtained in P(Ga)-X(x)-system, as functions of E

In the P(Ga)-X(x)-system, at T=0K and $N = N_{CDn(CDp)}(r_{P(Ga)}, x)$, our numerical results of n, κ, ε_1 and ε_2 are obtained from Equations (21, 20, 16), respectively, and expressed as functions of E [$\geq E_{CPE}(r_{P(Ga)}, x)$] and for given x, as those reported in Tables 3n and 3p in Appendix 1.

D. Variations of various optical coefficients, as functions of N

In the X(x)-system, at E=3.2 eV and T=20 K, for given $r_{d(a)}$ and x, and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of $\eta_{n(p)}(\gg 1, \text{degenerate case})$, $E_{gn1(gp1)}$, n, κ, ε_1 and ε_2, obtained as functions of N, being represented by the arrows: ↗ and ↘, as those tabulated in Tables 4n and 4p in Appendix 1.

E. Variations of various optical coefficients as functions of T

In the X(x)-system, at E=3.2 eV and $N = 10^{20} cm^{-3}$, for given $r_{d(a)}$ and x, and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of $\eta_{n(p)}(\gg 1, \text{degenerate case})$, $E_{gn1(gp1)}$, n, κ, ε_1 and ε_2, obtained as functions of T, being represented by the arrows: ↗ and ↘, as those tabulated in Tables 5n and 5p in Appendix 1.

CONCLUDING REMARKS

In the n(p)-type $\mathbf{X(x) \equiv CdS_{1-x}Te_x}$- crystalline alloy, by basing on our two recent works[1,2], for a given x, and with an increasing $r_{d(a)}$, the optical coefficients have been determined, as functions of the photon energy E, total impurity density N, the donor (acceptor) radius $r_{d(a)}$, concentration x, and temperature T.

Those results have been affected by **(i)** the important new $\varepsilon\left(r_{d(a)}, x\right)$-law, developed in Equations (8a, 8b), stating that, for a given x, due to the impurity-size effect, ε decreases (↘) with an increasing (↗) $r_{d(a)}$, and then by **(ii)** the generalized Mott critical d(a)-density defined in the metal-insulator transition (MIT), $N_{CDn(NDp)}(r_{d(a)}, x)$, as observed in Equations (8c, 9a).

Further, we also showed that $N_{CDn(NDp)}$ is just the density of carriers localized in exponential band tails, with a precision of the order of 2.84×10^{-7}, as that given in Table 4 of Ref.[1], according to a definition of the effective density of electrons (holes) given in parabolic conduction (valence) bands by: $N^*(N, r_{d(a)}, x) \equiv N - N_{CDn(NDp)}(r_{d(a)}, x)$, as defined in Eq. (9d).

In summary, due to the new $\varepsilon\left(r_{d(a)}, x\right)$-law and to the effective density of electrons (holes) given in parabolic conduction (valence) bands $N^*(N, r_{d(a)}, x)$, for a given x, and with an increasing $r_{d(a)}$, the numerical results of all the optical coefficients, obtained in appropriated physical conditions (E, N, T), and calculated by using Equations (15, 16, 20, 21), are investigated in Tables 1, 2, 3n, 3p, 4n, 4p, 5n, and 5p in Appendix 1.

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APPENDIX 1

Table 1. In the MIT-case, T=0K, N= $N_{CDn(p)}(r_{d(a)},x)$, and the critical photon energy $E_{CPE}=E=E_{gno(gpo)}(r_{d(a)},x)$, if $E=E_{gn1(gp1)}(r_{d(a)},x)=E_{CPE}(r_{d(a)},x)$, the numerical results of optical functions such as : $n_{MIT}(r_{d(a)},x)$, obtained from Eq. (21), and those of other ones: $\varepsilon_{1(MIT)}(r_{d(a)},x)$ and $R_{MIT}(r_{d(a)},x)$, from Eq. (16), decrease (↘) with increasing (↗) $r_{d(a)}$ and E_{CPE}.

Donor		S	Se	Te	Sn
r_d (nm) [4]	↗	0.104	0.114	0.132	0.140
At **x=0**,					
E_{CPE} in meV	↗	2580	2583	2605	2622
n_{MIT}	↘	2.401	2.364	2.164	2.057
$\varepsilon_{1(MIT)}$	↘	5.766	5.589	4.683	4.231
R_{MIT}	↘	0.170	0.164	0.135	0.119
At **x=0.5**,					
E_{CPE} in meV	↗	2100	2102	2116	2127
n_{MIT}	↘	2.761	2.724	2.521	2.415
$\varepsilon_{1(MIT)}$	↘	7.625	7.418	6.358	5.832
R_{MIT}	↘	0.219	0.214	0.187	0.172
At **x=1**,					
E_{CPE} in meV	↗	1620	1621	1629	1636
n_{MIT}	↘	3.119	3.081	2.876	2.769
$\varepsilon_{1(MIT)}$	↘	9.730	9.492	8.272	7.669
R_{MIT}	↘	0.265	0.260	0.234	0.220

Acceptor		Ga	Mg	In	Cd
r_a (nm)	↗	0.126	0.140	0.144	0.148
At **x=0**,					
E_{CPE} in meV	↗	2555	2576	2579	2580
n_{MIT}	↘	2.506	2.414	2.405	2.401
$\varepsilon_{1(MIT)}$	↘	6.281	5.830	5.782	5.766

R_{MIT}	↘	0.184	0.172	0.170	0.1697
At **x=0.5**,					
E_{CPE} in meV	↗	2078	2097	2099	2100
n_{MIT}	↘	2.867	2.775	2.765	2.761
$\varepsilon_{1(MIT)}$	↘	8.223	7.699	7.644	7.625
R_{MIT}	↘	0.233	0.221	0.220	0.219
At **x=1**,					
E_{CPE} in meV	↗	1601	1617	1619	1620
n_{MIT}	↘	3.227	3.133	3.123	3.119
$\varepsilon_{1(MIT)}$	↘	10.414	9.815	9.752	9.730
R_{MIT}	↘	0.277	0.266	0.265	0.2647

Table 2. Here, as $E \to \infty$, the numerical results of $n_{\infty}(r_{d(a)}, x)$, $\varepsilon_{1,\infty}(r_{d(a)}, x)$, $\sigma_{O,\infty}(r_{d(a)}, x)$, $\alpha_{\infty}(r_{d(a)}, x)$ and $R_{\infty}(r_{d(a)}, x)$ go to their appropriate limiting constants.

Donor		S	Se	Te	Sn
r_d (nm) [4]	↗	0.104	0.114	0.132	0.140
At **x=0**,					
n_{∞}	↘	1.7046	1.6693	1.4827	1.3867
$\varepsilon_{1,\infty}$	↘	2.906	2.7867	2.1983	1.9229
$\sigma_{O,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	7.7784	7.6173	6.7656	6.3275
$\propto_{\infty}$ in $(10^9 \times cm^{-1})$		2.160	2.160	2.160	2.160
R_{∞}	↘	0.068	0.063	0.038	0.026
At **x=0.5**,					
n_{∞}	↘	1.765	1.729	1.536	1.436
$\varepsilon_{1,\infty}$	↘	3.117	2.989	2.358	2.063
$\sigma_{O,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	8.056	7.889	7.007	6.554
$\propto_{\infty}$ in $(10^9 \times cm^{-1})$		2.160	2.160	2.160	2.160
R_{∞}	↘	0.077	0.071	0.045	0.032

At **x=1**,					
n_∞	↘	1.824	1.787	1.587	1.484
$\varepsilon_{1,\infty}$	↘	3.329	3.192	2.518	2.203
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	8.320	8.153	7.241	6.772
$\propto_\infty$ in $(10^9\times cm^{-1})$		2.160	2.160	2.160	2.160
R_∞	↘	0.085	0.080	0.051	0.038

Acceptor		Ga	Mg	In	Cd
r_a (nm)	↗	0.126	0.140	0.144	0.148
At **x=0**,					
n_∞	↘	1.794	1.716	1.707	1.705
$\varepsilon_{1,\infty}$	↘	3.218	2.944	2.915	2.906
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	8.186	7.829	7.791	7.778
$\propto_\infty$ in $(10^9\times cm^{-1})$		2.160	2.160	2.160	2.160
R_∞	↘	0.081	0.069	0.068	0.0679
At **x=0.5**,					
n_∞	↘	1.858	1.777	1.768	1.766
$\varepsilon_{1,\infty}$	↘	3.453	3.158	3.127	3.117
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	8.479	8.109	8.069	8.056
$\propto_\infty$ in $(10^9\times cm^{-1})$		2.160	2.160	2.160	2.160
R_∞	↘	0.090	0.078	0.077	0.120
At **x=1**,					
n_∞	↘	1.920	1.836	1.827	1.824
$\varepsilon_{1,\infty}$	↘	3.687	3.372	3.340	3.329
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	8.762	8.379	8.339	8.325
$\propto_\infty$ in $(10^9\times cm^{-1})$		2.160	2.160	2.160	2.160
R_∞	↘	0.099	0.087	0.086	0.085

Table 3n. In the P-X(x)-system, and at T=0K and $N = N_{CDn}(r_P,x)$, according to the MIT, our numerical results of n, κ, ε_1 and ε_2 are obtained from Equations (21, 20, 16), respectively, and expressed as functions of $E\,[\geq E_{CPE}(r_P,x)]$ and x, noting that (i) $\kappa = 0$ and $\varepsilon_2 = 0$ at $E = E_{CPE}(r_P,x)$, and $\kappa \to 0$ and $\varepsilon_2 \to 0$ as $E \to \infty$.

E in eV	n	κ	ε_1	ε_2
At x=0,				
$\mathbf{E_{CPE} = 2.5810}$	**2.3878**	**0**	**5.7015**	**0**
3	2.662	0.144	7.064	0.768
3.5	2.746	0.440	7.348	2.415
4	2.892	0.609	7.992	3.525
4.5	3.123	1.198	8.315	7.484
5	3.357	1.956	1.730	9.221
5.5	1.671	1.541	0.418	5.151
6	1.666	1.246	1.222	4.151
…				
$\mathbf{10^{22}}$	**1.6917**	**0**	**2.8620**	**0**
At x=0.5,				
$\mathbf{E_{CPE} = 2.1006}$	**2.7476**	**0**	**7.5493**	**0**
3	3.367	0.664	10.898	4.474
3.5	3.123	1.020	8.712	6.368
4	3.250	1.092	9.372	7.098
4.5	3.522	1.873	8.897	13.197
5	2.345	2.810	–2.399	13.177
5.5	1.427	2.090	–2.331	5.966
6	1.467	1.621	–0.475	4.756
…				
$\mathbf{10^{22}}$	**1.7522**	**0**	**3.0703**	**0**
At x=1,				
$\mathbf{E_{CPE} = 1.6204}$	**3.1053**	**0**	**9.6431**	**0**
2	3.396	0.217	11.487	1.477

2.5	4.015	0.293	16.038	2.352
3	4.105	1.563	14.405	12.836
3.5	3.380	1.840	8.042	12.437
4	3.519	1.714	9.449	12.065
4.5	3.862	2.698	7.633	20.842
5	2.209	3.818	–9.698	16.868
5.5	1.044	2.722	–6.321	5.684
6	1.154	2.045	–2.850	4.718
…				
10^{22}	**1.8107**	**0**	**3.2786**	**0**
E in eV	n	κ	ε_1	ε_2

Table 3p. In the Ga-X(x)-system, and at T=0K and $N = N_{CDp}(r_{Ga},x)$, according to the MIT, our numerical results of n, κ, ε_1 and ε_2 are obtained from Equations (21, 20, 16), respectively, and expressed as functions of $E\ [\geq E_{CPE}(r_{Ga},x)]$ and x, noting that (i) $\kappa = 0$ and $\varepsilon_2 = 0$ at $E = E_{CPE}(r_{Ga},x)$, and $\kappa \to 0$ and $\varepsilon_2 \to 0$ as $E \to \infty$.

E in eV	n	κ	ε_1	ε_2
At x=0,				
E_{CPE} =2.5551	**2.5062**	**0**	**6.2810**	**0**
3	2.798	0.162	7.802	0.910
3.5	2.868	0.465	8.012	2.667
4	3.012	0.632	8.676	3.807
4.5	3.245	1.231	9.013	7.987
5	2.458	1.998	2.052	9.824
5.5	1.761	1.568	0.639	5.523
6	1.757	1.265	1.486	4.445
…				
10^{22}	**1.7940**	**0**	**3.2185**	**0**

At x=0.5,				
E_{CPE} =2.0781	**2.8675**	**0**	**8.2229**	**0**
2.5	3.214	0.067	10.323	0.433
3	3.504	0.698	11.794	4.893
3.5	3.241	1.053	9.394	6.823
4	3.368	1.118	10.094	7.531
4.5	3.643	1.909	9.626	13.905
5	2.444	2.854	–2.170	13.950
5.5	1.515	2.118	–2.188	6.419
6	1.558	1.640	–0.261	5.109
…				
10^{22}	**1.8581**	**0**	**3.4527**	**0**
At x=1,				
E_{CPE} =1.6006	**3.2271**	**0**	**10.4143**	**0**
2	3.536	0.219	12.456	1.548
2.5	4.166	0.306	17.262	2.552
3	4.243	1.609	15.415	13.651
3.5	3.495	1.878	8.689	13.132
4	3.636	1.743	10.182	12.671
4.5	3.982	2.735	8.371	21.785
5	2.308	3.863	–9.595	17.830
5.5	1.132	2.750	–6.281	6.228
6	1.245	2.063	–2.706	5.140
…				
10^{22}	**1.9201**	**0**	**3.6870**	**0**
E in eV	n	κ	ε_1	ε_2

Table 4n. In the X(x)-system, at E=3.2 eV and T=20 K, for given r_d and x, and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of $\eta_n (\gg 1,\text{degenerate case})$, E_{gn1}, n, κ, ε_1 and ε_2, obtained as functions of N, being represented by the arrows: ↗ and ↘, noting that both η_n and E_{gn1} increase with increasing N.

N $(10^{18}\ cm^{-3})$	↗	15		26		60	100
x=0							
For $\mathbf{r_d = r_{Se}}$,							
$\eta_n \gg 1$	↗	226		334		594	840
E_{gn1} in eV	↗	2.909		3.078		3.492	3.887
n	↘	2.335		2.130		1.608	1.080
κ		0.063	↘	0.011	↗	0.063	0.350
ε_1	↘	5.448		4.537		2.582	1.045
ε_2		0.294	↘	0.047	↗	0.203	0.756
For $\mathbf{r_d = r_{Te}}$,							
$\eta_n \gg 1$	↗	211		322		585	833
E_{gn1} in eV	↗	2.914		3.090		3.513	3.915
n	↘	2.142		1.929		1.393	0.855
κ		0.061	↘	0.009	↗	0.073	0.379
ε_1	↘	4.585		3.722		1.936	0.587
ε_2		0.260	↘	0.035	↗	0.203	0.648
For $\mathbf{r_d = r_{Sn}}$,							
$\eta_n \gg 1$	↗	197		310		577	825
E_{gn1} in eV	↗	2.911		3.092		3.523	3.929
n	↘	2.049		1.830		1.285	0.740
κ		0.062	↘	0.0086	↗	0.077	0.394
ε_1	↘	4.197		3.349		1.644	0.392
ε_2		0.254	↘	0.031	↗	0.199	0.583
x=0.5							

For $\mathbf{r}_d = \mathbf{r}_{Se}$,

$\eta_n \gg 1$	↗	128	187	328	462
E_{gn1} in eV	↗	2.224	2.298	2.485	2.669
n	↘	3.168	3.089	2.883	2.675
κ	↘	0.705	0.603	0.379	0.209
ε_1	↘	9.539	9.178	8.171	7.113
ε_2	↘	4.469	3.725	2.184	1.117

For $\mathbf{r}_d = \mathbf{r}_{Te}$,

$\eta_n \gg 1$	↗	126	185	326	461
E_{gn1} in eV	↗	2.247	2.326	2.523	2.715
n	↘	2.950	2.865	2.648	2.428
κ	↘	0.672	0.566	0.340	0.174
ε_1	↘	8.251	7.891	6.895	5.867
ε_2	↘	3.968	3.246	1.798	0.845

For $\mathbf{r}_d = \mathbf{r}_{Sn}$,

$\eta_n \gg 1$	↗	123	183	325	459
E_{gn1} in eV	↗	2.261	2.342	2.544	2.704
n	↘	2.836	2.749	2.525	2.300
κ	↘	0.654	0.546	0.319	0.156
ε_1	↘	7.618	7.258	6.273	5.266
ε_2	↘	3.709	3.002	1.611	0.720

x=1

For $\mathbf{r}_d = \mathbf{r}_{Se}$,

$\eta_n \gg 1$	↗	93	135	236	332
E_{gn1} in eV	↗	1.593	1.612	1.673	1.744
n	↘	3.863	3.846	3.787	3.718
κ	↘	1.913	1.870	1.728	1.572
ε_1	↗	11.266	11.295	11.355 ↘	11.354

ε_2	↘	14.785	14.383	13.092	11.693
For $\mathbf{r_d} = \mathbf{r_{Te}}$,					
$\eta_n \gg 1$	↗	93	134.6	235.6	331
E_{gn1} in eV	↗	1.629	1.656	1.738	1.826
n	↘	3.630	3.603	3.524	3.437
κ	↘	1.830	1.766	1.584	1.399
ε_1	↗	9.828	9.865	9.909 ↘	9.856
ε_2	↘	13.286	12.728	11.168	9.621
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↗	92.5	134.2	235.4	331.3
E_{gn1} in eV	↗	1.647	1.679	1.770	1.866
n	↘	3.509	3.478	3.389	3.294
κ	↘	1.787	1.714	1.515	1.318
ε_1	↗	9.122	9.162	9.194 ↘	9.113
ε_2	↘	12.541	11.923	10.271	8.686
N $(10^{18}\ cm^{-3})$	↗	15	26	60	100

Table 4p. In the X(x)-system, at E=3.2 eV and T=20 K, for given r_d and x, and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of $\eta_p (\gg 1, \text{degenerate case})$, E_{gp1}, n, κ, ε_1 and ε_2, obtained as functions of N, being represented by the arrows: ↗ and ↘, noting that both η_p and E_{gp1} increase with increasing N.

N $(10^{18}\ cm^{-3})$	↗	75	80	85	100
		x=0			
For $\mathbf{r_a} = \mathbf{r_{Ga}}$,					
$\eta_p \gg 1$	↗	115	133	150	196
E_{gp1} in eV	↗	1.788	1.818	1.847	1.924
n	↘	3.681	3.652	3.623	3.546

κ	↘	1.477	1.415	1.357	1.207
ε_1	↘	11.373	11.334	11.288	11.117
ε_2	↘	10.879	10.333	9.837	8.560
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↗	22	55	79	138
E_{gp1} in eV	↗	1.652	1.706	1.747	1.844
n	↘	3.728	3.676	3.636	3.539
κ	↘	1.776	1.654	1.565	1.362
ε_1	↘	10.744	10.774	10.769	10.671
ε_2	↘	13.243	12.163	11.379	9.642
For $\mathbf{r_a} = \mathbf{r_{Cd}}$,					
$\eta_p \gg 1$	↗	15	51	76	135
E_{gp1} in eV	↗	1.642	1.700	1.742	1.841
n	↘	3.735	3.679	3.638	3.540
κ	↘	1.799	1.667	1.575	1.369
ε_1		10.712	↗ 10.752	↘ 10.751	10.657
ε_2	↘	13.443	12.269	11.460	9.693
			x=0.5		
For $\mathbf{r_a} = \mathbf{r_{Ga}}$,					
$\eta_p \gg 1$	↗	204	227	249	308
E_{gp1} in eV	↗	2.417	2.456	2.492	2.593
n	↘	3.088	3.045	3.005	2.891
κ	↘	0.454	0.411	0.371	0.273
ε_1	↘	9.329	9.106	8.891	8.282
ε_2	↘	2.803	2.501	2.232	1.577
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↗	122	150	176	245
E_{gp1} in eV	↗	2.300	2.348	2.392	2.508

n	↘	3.127	3.074	3.026	2.897
κ	↘	0.601	0.538	0.484	0.355
ε_1	↘	9.415	9.163	8.924	8.268
ε_2	↘	3.757	3.310	2.931	2.056

For $\mathbf{r_a} = \mathbf{r_{Cd}}$,

$\eta_p \gg 1$	↗	118	147	173	243
E_{gp1} in eV	↗	2.294	2.343	2.387	2.505
n	↘	3.130	3.077	3.028	2.898
κ	↘	0.608	0.544	0.489	0.358
ε_1	↘	9.425	9.170	8.931	8.272
ε_2	↘	3.805	3.350	2.964	2.078

x=1

For $\mathbf{r_a} = \mathbf{r_{Ga}}$,

$\eta_p \gg 1$	↗	168	184	198	239
E_{gp1} in eV	↗	1.876	1.902	1.926	1.995
n	↘	3.720	3.694	3.670	3.599
κ	↘	1.298	1.249	1.202	1.076
ε_1	↘	12.152	12.088	12.020	11.798
ε_2	↘	9.663	9.230	8.826	7.748

For $\mathbf{r_a} = \mathbf{r_{In}}$,

$\eta_p \gg 1$	↗	123	141	157	203
E_{gp1} in eV	↗	1.820	1.850	1.877	1.953
n	↘	3.683	3.654	3.626	3.550
κ	↘	1.411	1.351	1.297	1.152
ε_1	↘	11.576	11.525	11.469	11.272
ε_2	↘	10.393	9.876	9.404	8.181

For $\mathbf{r_a} = \mathbf{r_{Cd}}$,

$\eta_p \gg 1$	↗	122	139	156	201

E_{gp1} in eV	↗	1.818	1.847	1.875	1.951
n	↘	3.683	3.653	3.625	3.548
κ	↘	1.416	1.356	1.301	1.155
ε_1	↘	11.558	11.508	11.452	11.256
ε_2	↘	10.428	9.907	9.431	8.201

N (10^{18} cm^{-3})	↗	15	26	60	100

Table 5n. In the X(x)-system, at E=3.2 eV and $N = 10^{20} cm^{-3}$, for given r_d and x, and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of $\eta_n (\gg 1$, degenerate case), E_{gn1}, n, κ, ε_1 and ε_2, obtained as functions of T, being represented by the arrows: ↗ and ↘, noting that both η_n and E_{gn1} decrease with increasing T.

T in K	↗	20	50	100	300
			x=0		
For $\mathbf{r_d} = \mathbf{r_{Se}}$,					
$\eta_n \gg 1$	↘	840	336	168	56
E_{gn1} in eV	↘	3.887	3.877	3.853	3.729
n	↗	1.080	1.094	1.126	1.295
κ	↘	0.350	0.340	0.316	0.207
ε_1	↗	1.045	1.080	1.169	1.633
ε_2	↘	0.756	0.744	0.713	0.537
For $\mathbf{r_d} = \mathbf{r_{Te}}$,					
$\eta_n \gg 1$	↘	833	333	166	55
E_{gn1} in eV	↘	3.915	3.905	3.881	3.757
n	↗	0.855	0.868	0.901	1.070
κ	↘	0.379	0.369	0.344	0.230
ε_1	↗	0.587	0.618	0.694	1.092
ε_2	↘	0.648	0.641	0.621	0.493
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					

$\eta_n \gg 1$	↘	825	330	165	55
E_{gn1} in eV	↘	3.929	3.919	3.895	3.771
n	↗	0.740	0.753	0.786	0.955
κ	↘	0.394	0.384	0.359	0.242
ε_1	↗	0.392	0.420	0.489	0.854
ε_2	↘	0.583	0.578	0.564	0.462

x=0.5

For $\mathbf{r_d} = \mathbf{r_{Se}}$,

$\eta_n \gg 1$	↘	462	185	92	31
E_{gn1} in eV	↘	2.669	2.661	2.642	2.540
n	↗	2.675	2.684	2.706	2.821
κ	↗	0.209	0.215	0.231	0.322
ε_1	↗	7.113	7.159	7.272	7.857
ε_2	↗	1.117	1.155	1.250	1.819

For $\mathbf{r_d} = \mathbf{r_{Te}}$,

$\eta_n \gg 1$	↘	461	184	92	31
E_{gn1} in eV	↘	2.715	2.707	2.688	2.587
n	↗	2.428	2.437	2.460	2.576
κ	↗	0.174	0.180	0.194	0.279
ε_1	↗	5.867	5.909	6.014	6.558
ε_2	↗	0.845	0.876	0.956	1.436

For $\mathbf{r_d} = \mathbf{r_{Sn}}$,

$\eta_n \gg 1$	↘	459	184	92	30.6
E_{gn1} in eV	↘	2.740	2.732	2.713	2.612
n	↗	2.300	2.309	2.332	2.448
κ	↗	0.156	0.162	0.176	0.256
ε_1	↗	5.266	5.306	5.407	5.928
ε_2	↗	0.720	0.748	0.820	1.256

x=1

For $\mathbf{r_d} = \mathbf{r_{Se}}$,					
$\eta_n \gg 1$	↘	332	133	66	22
E_{gn1} in eV	↘	1.744	1.737	1.722	1.644
n	↗	3.718	3.724	3.739	3.814
κ	↗	1.572	1.585	1.618	1.794
ε_1	↗	11.354	11.357	11.362 ↘	11.334
ε_2	↗	11.693	11.809	12.101	13.690
For $\mathbf{r_d} = \mathbf{r_{Te}}$,					
$\eta_n \gg 1$	↘	331	132.6	66.3	22
E_{gn1} in eV	↘	1.826	1.820	1.805	1.726
n	↗	3.437	3.443	3.458	3.535
κ	↗	1.399	1.412	1.443	1.609
ε_1	↗	9.856	9.863	9.877	9.908
ε_2	↗	9.621	9.823	9.980	11.380
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↘	331	132.5	66.2	22
E_{gn1} in eV	↘	1.866	1.860	1.845	1.767
n	↗	3.294	3.300	3.315	3.393
κ	↗	1.318	1.330	1.360	1.522
ε_1	↗	9.113	9.121	9.140	9.194
ε_2	↗	8.686	8.781	9.021	10.330
T in K	↗	20	50	100	300

Table 5p. In the X(x)-system, at E=3.2 eV and $N = 10^{20} cm^{-3}$, for given r_a and x, and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of $\eta_p (\gg 1$, degenerate case), E_{gp1}, n, κ, ε_1 and ε_2, obtained as functions of T, being represented by the arrows: ↗ and ↘, noting that both η_p and E_{gp1} decrease with increasing T.

T in K	↗	20	50	100	300
x=0					
For $\mathbf{r_a = r_{Ga}}$,					
$\eta_p \gg 1$	↘	501	200	100	33
E_{gp1} in eV	↘	3.405	3.394	3.371	3.247
n	↗	1.845	1.858	1.888	2.046
κ	↘	0.031	0.028	0.022	0.002
ε_1	↗	3.404	3.450	3.566	4.186
ε_2	↘	0.115	0.105	0.082	0.007
For $\mathbf{r_a = r_{In}}$,					
$\eta_p \gg 1$	↘	351	140	70	23
E_{gp1} in eV	↘	3.173	3.163	3.139	3.015
n	↗	2.051	2.063	2.093	2.245
κ	↗	0.0005	0.0009	0.003	0.025
ε_1	↗	4.207	4.257	4.380	5.042
ε_2	↗	0.002	0.004	0.011	0.114
For $\mathbf{r_a = r_{Cd}}$,					
$\eta_p \gg 1$	↘	345	138	69	23
E_{gp1} in eV	↘	3.163	3.153	3.129	3.005
n	↗	2.061	2.073	2.102	2.255
κ	↗	0.001	0.0016	0.0037	0.028
ε_1	↗	4.246	4.296	4.420	5.083
ε_2	↗	0.004	0.0066	0.015	0.127
x=0.5					

For $\mathbf{r_a} = \mathbf{r_{Ga}}$,

$\eta_p \gg 1$	↘	308	123	62	20
E_{gp1} in eV	↘	2.593	2.585	2.566	2.464
n	↗	2.891	2.900	2.922	3.036
κ	↗	0.273	0.280	0.298	0.401
ε_1	↗	8.282	8.330	8.449	9.055
ε_2	↗	1.577	1.623	1.741	2.435

For $\mathbf{r_a} = \mathbf{r_{In}}$,

$\eta_p \gg 1$	↘	245	98	49	16
E_{gp1} in eV	↘	2.508	2.500	2.481	2.379
n	↗	2.897	2.906	2.928	3.040
κ	↗	0.355	0.363	0.383	0.500
ε_1	↗	8.268	8.314	8.426	8.995
ε_2	↗	2.056	2.101	2.246	3.040

For $\mathbf{r_a} = \mathbf{r_{Cd}}$,

$\eta_p \gg 1$	↘	243	97	48	16
E_{gp1} in eV	↘	2.505	2.497	2.477	2.375
n	↗	2.898	2.907	2.929	3.042
κ	↗	0.358	0.367	0.387	0.504
ε_1	↗	8.272	8.318	8.429	8.997
ε_2	↗	2.078	2.132	2.269	3.067

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x=1

For $\mathbf{r_a} = \mathbf{r_{Ga}}$,

$\eta_p \gg 1$	↘	239	96	48	20.6
E_{gp1} in eV	↘	1.995	1.989	1.974	2.128
n	↗	3.600	3.606	3.621	3.434
κ	↗	1.076	1.087	1.114	0.852
ε_1	↗	11.798	11.820	11.871	11.070

ε_2	↗	7.748	7.840	8.071	5.851
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↘	203	81	40	13.45
E_{gp1} in eV	↘	1.953	1.947	1.932	1.853
n	↗	3.550	3.556	3.571	3.651
κ	↗	1.152	1.164	1.192	1.345
ε_1	↗	11.272	11.290	11.333	11.519
ε_2	↗	8.181	8.275	8.513	9.818
For $\mathbf{r_a} = \mathbf{r_{Cd}}$,					
$\eta_p \gg 1$	↘	201	80	40	13.35
E_{gp1} in eV	↘	1.951	1.945	1.930	1.851
n	↗	3.548	3.555	3.570	3.649
κ	↗	1.155	1.167	1.195	1.348
ε_1	↗	11.256	11.274	11.317	11.501
ε_2	↗	8.201	8.296	8.533	9.840
T in K	↗	20	50	100	300