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OPTICAL COEFFICIENTS IN THE N(P)-TYPE DEGENERATE CDS(1-X) SE(X)-CRYSTALLINE ALLOY, DUE TO THE NEW STATIC DIELECTRIC CONSTANT-LAW AND THE GENERALIZED MOTT CRITERIUM IN THE METAL-INSULATOR TRANSITION

Prof. Dr. Huynh Van Cong*

Université de Perpignan Via Domitia, Laboratoire de Mathématiques et Physique (LAMPS), EA 4217, Département de Physique, 52, Avenue Paul Alduy, F-66 860 Perpignan, France.

*Corresponding Author
Prof. Dr. Huynh Van Cong
Université de Perpignan Via Domitia, Laboratoire de Mathématiques et Physique (LAMPS), EA 4217, Département de Physique, 52, Avenue Paul Alduy, F-66 860 Perpignan, France.

ABTRACT

In the n(p)-type $CdS_{1-x}Se_x$- 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 ($\searrow$) with an increasing ($\nearrow$) $r_{d(a)}$, 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 2.88×10^{-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: $CdS_{1-x}Se_x$- crystalline alloy; impurity-size effect; Mott critical impurity density in the MIT, optical coefficents.

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 $X(x) \equiv CdS_{1-x}Se_x$- crystalline alloy, with $0 \leq x \leq 1$, 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 $n^+(p^+) - p(n)$ $X(x) \equiv CdS_{1-x}Se_x$- 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:

$$m_{c(v)}(x)/m_o = 0.11(0.45) \times x + 0.197 (0.801) \times (1 - x) \tag{1}$$

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

$$\varepsilon_o(x) = 10.2 \times x + 9 \times (1 - x). \tag{2}$$

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

$$E_{go}(x) = 1.84 \times x + 2.58 \times (1 - x). \tag{3}$$

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

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

and then, the isothermal bulk modulus, by:

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

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: $\frac{d}{dV}(\frac{d\sigma}{dV}) = \frac{B}{V}$. Then, by an integration, one gets:

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

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: $\pm \left[\Delta\sigma(r_{d(a)}, x)\right]_{n(p)}$,

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

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

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

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

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

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

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

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 $\varepsilon(r_{d(a)}, x) = \dfrac{\varepsilon_o(x)}{\sqrt{1 - \left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3}} \geq \varepsilon_o(x)$, 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 $\varepsilon(r_{d(a)}, x)$-law**,

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

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:

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

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:

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

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

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

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:

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

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

Furthermore, by using $\mathbf{M_{n(p)} = 0.25}$, according to the empirical Heisenberg parameter $\mathcal{H}_{n(p)} = 0.47137$, 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 2.88×10^{-7}. Therefore, the density of electrons (holes) given in parabolic conduction (valence) bands can be defined, as that given in compensated materials, by:

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

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

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

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

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:

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

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:

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

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

$F(u) = au^{\frac{2}{3}}\left(1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}}\right)^{-\frac{2}{3}}$, $a = [(3\sqrt{\pi}/4) \times u]^{2/3}$, $b = \frac{1}{8}\left(\frac{\pi}{a}\right)^2$, $c = \frac{62.3739855}{1920}\left(\frac{\pi}{a}\right)^4$, 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) $\frac{E_{Fn}(u \ll 1)}{k_B T}(\frac{-E_{Fp}(u \ll 1)}{k_B T}) \ll -1$, 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:

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

$$\Delta E_{gn}(N, r_d, x) \simeq a_1 \times \frac{\varepsilon_o(x)}{\varepsilon(r_d,x)} \times N_r^{1/3} + a_2 \times \frac{\varepsilon_o(x)}{\varepsilon(r_d,x)} \times N_r^{\frac{1}{3}} \times (2.503 \times [-E_{cn}(r_{sn}) \times r_{sn}]) + a_3 \times$$

$$\left[\frac{\varepsilon_o(x)}{\varepsilon(r_d,x)}\right]^{5/4} \times \sqrt{\frac{m_v}{m_r}} \times N_r^{1/4} + a_4 \times \sqrt{\frac{\varepsilon_o(x)}{\varepsilon(r_d,x)}} \times N_r^{1/2} \times 2 + a_5 \times \left[\frac{\varepsilon_o(x)}{\varepsilon(r_d,x)}\right]^{\frac{3}{2}} \times N_r^{\frac{1}{6}}$$

$$, N_r \equiv \left(\frac{N^*}{N_{CDn(r_d,x)}}\right), \tag{14n}$$

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:

$$\Delta E_{gp}(N, r_a, x) \simeq a_1 \times \frac{\varepsilon_o(x)}{\varepsilon(r_a,x)} \times N_r^{1/3} + a_2 \times \frac{\varepsilon_o(x)}{\varepsilon(r_a,x)} \times N_r^{\frac{1}{3}} \times (2.503 \times [-E_{cp}(r_{sp}) \times r_{sp}]) + a_3 \times$$

$$\left[\frac{\varepsilon_o(x)}{\varepsilon(r_a,x)}\right]^{5/4} \times \sqrt{\frac{m_c}{m_r}} \times N_r^{1/4} + 2a_4 \times \sqrt{\frac{\varepsilon_o(x)}{\varepsilon(r_a,x)}} \times N_r^{1/2} + a_5 \times \left[\frac{\varepsilon_o(x)}{\varepsilon(r_a,x)}\right]^{\frac{3}{2}} \times N_r^{\frac{1}{6}}$$

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

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 $a_5 = 9.8 \times 10^{-5}(eV)$.

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:

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

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]

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

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

Here, $-q$, $\hbar$, $|v(E)|$, ω, $\varepsilon_{free\ space}$, 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:

$$R(E, N, r_{d(a)}, x, T) = \frac{[n(E)-1]^2 + \kappa(E)^2}{[n(E)+1]^2 + \kappa(E)^2}. \tag{17}$$

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: $E_{gn1(gp1)}(N, r_{d(a)}, x, T) = E_{gn1(gp1)}$, for a presentation simplicity.

Then, one has:

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

$$J_{n(p)}(E, N, r_{d(a)}, x, T) = \frac{1}{2\pi^2} \times \left(\frac{2m_r}{\hbar^2}\right)^{3/2} \times \frac{(E-E_{gn1(gp1)})^{a-(1/2)}}{E_{gni(gpi)}^{a-1}} = \frac{1}{2\pi^2} \times \left(\frac{2m_r}{\hbar^2}\right)^{3/2} \times (E - E_{gn1(gp1)})^{1/2}, \text{ for a=1}, \tag{18}$$

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

$$J_{n(p)}(E, N, r_{d(a)}, x, T) = \frac{1}{2\pi^2} \times \left(\frac{2m_r}{\hbar^2}\right)^{3/2} \times \frac{(E-E_{gn1(gp1)})^{a-(1/2)}}{E_{gni(gpi)}^{a-1}} = \frac{1}{2\pi^2} \times \left(\frac{2m_r}{\hbar^2}\right)^{3/2} \times \frac{(E-E_{gn1(gp1)})^2}{E_{gni(gpi)}^{3/2}}, \text{ for a=5/2}. \tag{19}$$

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:

$$G(E) \equiv \sum_{i=1}^{4} \frac{A_i}{E^2 - B_i E + C_i} \text{ and } F(E) \equiv \sum_{i=1}^{4} \frac{A_i}{E^2 \times (1 + 10^{-4} \times \frac{E}{6}) - B_i E + C_i}, \text{ we propose:}$$

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

$$= F(E) \times \left(E^* \equiv E - E_{gn1(gp1)}\right)^2, \text{ for } E \geq 2.3 \text{ eV}, \tag{20}$$

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,

$$n(E, N, r_{d(a)}, x, T) = n_\infty(r_{d(a)}, x) + \sum_{i=1}^{4} \frac{X_i(E_{gn1(gp1)}) \times E + Y_i(E_{gn1(gp1)})}{E^2 - B_i E + C_i}. \tag{21}$$

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

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 $X(x) \equiv CdS_{1-x}Se_x$- 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 coefficents, obtained as E → ∞

In Eq. (21), at any T, the choice of the real refraction index:

$$n(E \to \infty, r_{d(a)}, x, T) = n_\infty(r_{d(a)}, x) = \sqrt{\varepsilon(r_{d(a)}, x)} \times \frac{\omega_T}{\omega_L} \quad , \quad \omega_T = 5.1 \times 10^{13} \ s^{-1} \quad [5] \quad \text{and}$$

$\omega_L = 8.9755 \times 10^{13} \ s^{-1}$, 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 $\varepsilon_{1,\infty}(r_{d(a)}, x)$, $\sigma_{0,\infty}(r_{d(a)}, x)$, $\alpha_\infty(r_{d(a)}, x)$ 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 $N = 10^{20} \text{cm}^{-3}$, 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 $X(x) \equiv CdS_{1-x}Se_x$- 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 ($\searrow$) with an increasing ($\nearrow$) $r_{d(a)}$, and then by **(ii)** the generalized Mott critical d(a)-density defined in the metal-insulator transition (MIT), $N_{CDn(NDp)}\left(r_{d(a)}, x\right)$, 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 2.88×10^{-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: $N^{*}(N, r_{d(a)}, x) \equiv N - N_{CDn(NDp)}\left(r_{d(a)}, x\right)$, 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.

ACKNOWLEDGMENT

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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 ($\searrow$) with increasing ($\nearrow$) $r_{d(a)}$ and E_{CPE}.

Donor		S	Se	Te	Sn
r_d (nm) [4]	$\nearrow$	0.104	0.114	0.132	0.140

At **x=0**,					
E_{CPE} in meV	$\nearrow$	2580	2583	2605	2622
n_{MIT}	$\searrow$	2.401	2.364	2.164	2.057
$\varepsilon_{1(MIT)}$	$\searrow$	5.766	5.589	4.683	4.231
R_{MIT}	$\searrow$	0.170	0.164	0.135	0.119
At **x=0.5**,					
E_{CPE} in meV	$\nearrow$	2210	2212	2227	2239
n_{MIT}	$\searrow$	2.688	2.650	2.448	2.341
$\varepsilon_{1(MIT)}$	$\searrow$	7.224	7.023	5.993	5.481
R_{MIT}	$\searrow$	0.209	0.204	0.176	0.161
At **x=1**,					
E_{CPE} in meV	$\nearrow$	1840	1841	1851	1858
n_{MIT}	$\searrow$	2.972	2.934	2.729	2.622
$\varepsilon_{1(MIT)}$	$\searrow$	8.836	8.609	7.450	6.878
R_{MIT}	$\searrow$	0.246	0.242	0.215	0.201

Acceptor		Ga	Mg	In	Cd
r_a (nm)	$\nearrow$	0.126	0.140	0.144	0.148

At **x=0**,					
E_{CPE} in meV	$\nearrow$	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	↗	2193	2208	2209	2210
n_{MIT}	↘	2.791	2.701	2.691	2.688
$\varepsilon_{1(MIT)}$	↘	7.788	7.294	7.241	7.224
R_{MIT}	↘	0.223	0.211	0.210	0.209

At **x=1**,

E_{CPE} in meV	↗	1829	1838	1839.6	1840
n_{MIT}	↘	3.074	2.985	2.976	2.972
$\varepsilon_{1(MIT)}$	↘	9.452	8.912	8.855	8.836
R_{MIT}	↘	0.259	0.248	0.247	0.246

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**,

		S	Se	Te	Sn
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
α_∞ 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**,

		S	Se	Te	Sn
n_∞	↘	1.760	1.724	1.531	1.432
$\varepsilon_{1,\infty}$	↘	3.099	2.972	2.345	2.051

$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	8.033	7.867	6.987	6.535
α_∞ in $(10^9 \times cm^{-1})$		2.160	2.160	2.160	2.160
R_∞	↘	0.076	0.071	0.044	0.031

At **x=1,**

n_∞	↘	1.815	1.777	1.578	1.476
$\varepsilon_{1,\infty}$	↘	3.293	3.158	2.491	2.179
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	8.281	8.109	7.202	6.736
α_∞ in $(10^9 \times cm^{-1})$		2.160	2.160	2.160	2.160
R_∞	↘	0.084	0.078	0.050	0.037

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
α_∞ 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_∞	↘	1.853	1.772	1.763	1.760
$\varepsilon_{1,\infty}$	↘	3.433	3.140	3.110	3.099
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	8.455	8.056	8.046	8.033
α_∞ in $(10^9 \times cm^{-1})$		2.160	2.160	2.160	2.160
R_∞	↘	0.089	0.077	0.076	0.0759

At **x=1**,

n_∞	↘	1.910	1.826	1.818	1.815
$\varepsilon_{1,\infty}$	↘	3.648	3.336	3.304	3.293
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$ ↘		8.715	8.334	8.294	8.281
α_∞ in $(10^9 \times cm^{-1})$		2.160	2.160	2.160	2.160
R_∞	↘	0.098 0.085	0.084	0.0838	

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,				
$E_{CPE} = 2.5810$	**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
…				
10^{22}	**1.6917**	**0**	**2.8620**	**0**
At x=0.5,				
$E_{CPE} = 2.2107$	**2.6740**	**0**	**7.1504**	**0**
3	3.212	0.512	10.053	3.287
3.5	3.056	0.865	8.588	5.290
4	3.185	0.969	9.204	6.173
4.5	3.445	1.705	8.957	11.749

E in eV	n	κ	ε_1	ε_2
5	2.367	2.601	−1.161	12.312
5.5	1.504	1.957	−1.567	5.887
6	1.531	1.531	0.0021	4.688
…				
10^{22}	**1.7472**	**0**	**3.0528**	**0**

At x=1,

E in eV	n	κ	ε_1	ε_2
$E_{CPE} = 1.8404$	2.9585	0	8.7528	0
2	3.067	0.171	9.381	1.047
2.5	3.573	0.165	12.739	1.177
3	3.780	1.104	13.067	8.349
3.5	3.294	1.434	8.793	9.448
4	3.424	1.412	9.731	9.667
4.5	3.730	2.302	8.619	17.173
5	2.303	3.337	−5.830	15.372
5.5	1.254	2.422	−4.295	6.074
6	1.328	1.844	−1.637	4.900
…				
10^{22}	**1.8010**	**0**	**3.2436**	**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,

$E_{CPE} = 2.1929$	**2.7907**	**0**	**7.7881**	**0**
2.5	3.026	0.036	9.156	0.216
3	3.341	0.535	10.879	3.576
3.5	3.172	0.889	9.269	5.643
4	3.300	0.988	9.916	6.525
4.5	3.562	1.732	9.689	12.340
5	2.469	2.634	-0.843	13.005
5.5	1.597	1.978	-1.362	6.318
6	1.626	1.545	0.257	5.025
…				
10^{22}	**1.8528**	**0**	**3.4331**	**0**

At x=1,

$E_{CPE} = 1.8291$	**3.0744**	**0**	**9.4522**	**0**
2	3.192	0.175	10.158	1.117
2.5	3.703	0.170	13.684	1.262
3	3.905	1.126	13.979	8.795
3.5	3.407	1.454	9.496	9.907
4	3.538	1.426	10.481	10.093
4.5	3.846	2.321	9.403	17.856
5	2.407	3.361	-5.500	16.183

5.5	1.352	2.437	−4.112	6.590
6	1.428	1.854	−1.399	5.298
…				
10^{22}	1.9099	0	3.6476	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.

$N\ (10^{18}\ \mathrm{cm}^{-3})$ ↗	15	26	60	100
		x=0		
For $r_d = r_{Se}$,				
$\eta_n \gg 1$ ↗	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 $r_d = r_{Te}$,				
$\eta_n \gg 1$ ↗	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 $r_d = r_{Sn}$,				
$\eta_n \gg 1$ ↗	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 $r_d = r_{Se}$,

$\eta_n \gg 1$	↗	128	186	328	462
E_{gn1} in eV	↗	2.341	2.416	2.608	2.795
n	↘	3.038	2.955	2.740	2.523
κ	↘	0.547	0.455	0.260	0.121
ε_1	↘	8.928	8.523	7.441	6.353
ε_2	↘	3.324	2.688	1.423	0.612

For $r_d = r_{Te}$,

$\eta_n \gg 1$	↗	125	184	326	460
E_{gn1} in eV	↗	2.363	2.443	2.644	2.839
n	↘	2.821	2.732	2.506	2.279
κ	↘	0.519	0.424	0.229	0.096
ε_1	↘	7.687	7.286	6.228	5.185
ε_2	↘	2.930	2.320	1.148	0.439

For $r_d = r_{Sn}$,

$\eta_n \gg 1$	↗	122	181	324	459
E_{gn1} in eV	↗	2.376	2.458	2.664	2.863
n	↘	2.707	2.616	2.384	2.152
κ	↘	0.503	0.407	0.213	0.084
ε_1	↘	7.077	6.679	5.638	4.622
ε_2	↘	2.727	2.132	1.014	0.361

x=1

For $r_d = r_{Se}$,

$\eta_n \gg 1$	↗	93	135	236	332
E_{gn1} in eV	↗	1.849	1.878	1.962	2.052
n	↘	3.604	3.575	3.490	3.398
κ	↘	1.352	1.295	1.136	0.977
ε_1	↘	11.161	11.105	10.891	10.591
ε_2	↘	9.749	9.260	7.928	6.640

For $r_d = r_{Te}$,

$\eta_n \gg 1$	↗	92	134	235	331
E_{gn1} in eV	↗	1.880	1.916	2.016	2.119
n	↘	3.375	3.338	3.236	3.129
κ	↘	1.292	1.222	1.039	0.866
ε_1	↘	9.721	9.651	9.394	9.040
ε_2	↘	8.723	8.159	6.727	5.417

For $r_d = r_{Sn}$,					
$\eta_n \gg 1$	↗	92	134	235	331
E_{gn1} in eV	↗	1.896	1.936	2.043	2.153
n	↘	3.256	3.216	3.106	2.991
κ	↘	1.260	1.184	0.991	0.812
ε_1	↘	9.015	8.939	8.662	8.286
ε_2	↘	8.204	7.615	6.158	4.858
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	95	100

x=0

For $r_a = r_{Ga}$,							
$\eta_p \gg 1$	↗	295		341		464	501
E_{gp1} in eV	↗	3.052		3.131		3.341	3.405
n	↘	2.286		2.190		1.927	1.845
κ		0.016	↘	0.0035	↗	0.015	0.031
ε_1	↘	5.227		4.796		3.713	3.404
ε_2		0.074	↘	0.015	↗	0.057	0.115

For $r_a = r_{In}$,					
$\eta_p \gg 1$	↗	57	140	306	351
E_{gp1} in eV	↗	2.671	2.813	3.096	3.173
n	↘	2.651	2.487	2.147	2.051
κ	↘	0.207	0.111	0.008	0.0005
ε_1	↘	6.987	6.171	4.608	4.207
ε_2	↘	1.100	0.553	0.034	0.002

For $r_a = r_{Cd}$,					
$\eta_p \gg 1$	↗	39	130	299	345
E_{gp1} in eV	↗	2.643	2.796	3.085	3.163
n	↘	2.681	2.503	2.157	2.061
κ	↘	0.230	0.121	0.001	0.001
ε_1	↘	7.133	6.251	4.652	4.246

ε_2	↘	1.233	0.605	0.042	0.004

x=0.5

For $r_a = r_{Ga}$,

$\eta_p \gg 1$	↗	306	324	378	395
E_{gp1} in eV	↗	2.698	2.730	2.820	2.848
n	↘	2.765	2.729	2.629	2.590
κ	↘	0.186	0.164	0.107	0.092
ε_1	↘	7.611	7.419	6.873	6.701
ε_2	↘	1.031	0.893	0.562	0.475

For $r_a = r_{In}$,

$\eta_p \gg 1$	↗	277	297	352	369
E_{gp1} in eV	↗	2.667	2.701	2.794	2.823
n	↘	2.711	2.673	2.565	2.530
κ	↘	0.210	0.185	0.122	0.105
ε_1	↘	7.307	7.112	6.562	6.389
ε_2	↘	1.139	0.988	0.626	0.531

For $r_a = r_{Cd}$,

$\eta_p \gg 1$	↗	276	296	351	368.6
E_{gp1} in eV	↗	2.666	2.699	2.793	2.822
n	↘	2.710	2.672	2.563	2.528
κ	↘	0.211	0.186	0.123	0.105
ε_1	↘	7.299	7.104	6.554	6.381
ε_2	↘	1.144	0.992	0.629	0.534

x=1

For $r_a = r_{Ga}$,

$\eta_p \gg 1$	↗	258	270	306	317
E_{gp1} in eV	↗	2.235	2.256	2.314	2.333
n	↘	3.337	3.315	3.253	3.232
κ	↘	0.690	0.661	0.582	0.557
ε_1	↘	10.662	10.556	10.241	10.137
ε_2	↘	4.603	4.383	3.785	3.605

For $r_a = r_{In}$,

$\eta_p \gg 1$	↗	252	264	300	312
E_{gp1} in eV	↗	2.239	2.259	2.318	2.337
n	↘	3.242	3.220	3.156	3.135
κ	↘	0.685	0.656	0.576	0.552
ε_1	↘	10.039	9.936	9.628	9.526
ε_2	↘	4.442	4.225	3.638	3.461

For $r_a = r_{Cd}$,

$\eta_p \gg 1$	↗	251.6	264	300	311.7
E_{gp1} in eV	↗	2.2387	2.259	2.318	2.337
n	↘	3.239	3.217	3.153	3.132
κ	↘	0.685	0.656	0.576	0.552
ε_1	↘	10.020	9.916	9.608	9.507
ε_2	↘	4.437	4.221	3.633	3.456
$N\,(10^{18}\,\mathrm{cm}^{-3})$	↗	75	80	95	100

Table 5n. In the X(x)-system, at E=3.2 eV and $N = 10^{20}\,\mathrm{cm}^{-3}$, for given r_d and x, and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of $\eta_n\,(\gg 1, \text{degenerate case})$, 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 $r_d = r_{Se}$,					
$\eta_n \gg 1$	↘	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 $r_d = r_{Te}$,					
$\eta_n \gg 1$	↘	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 $r_d = r_{Sn}$,					
$\eta_n \gg 1$	↘	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 $r_d = r_{Se}$,

$\eta_n \gg 1$	↘	462	185	92	31
E_{gn1} in eV	↘	2.795	2.788	2.768	2.667
n	↗	2.523	2.533	2.555	2.673
κ	↗	0.121	0.126	0.138	0.211
ε_1	↗	6.353	6.399	6.512	7.100
ε_2	↗	0.611	0.638	0.706	1.126

For $r_d = r_{Te}$,

$\eta_n \gg 1$	↘	460	184	92	31
E_{gn1} in eV	↘	2.839	2.831	2.812	2.711
n	↗	2.279	2.288	2.311	2.429
κ	↗	0.096	0.101	0.111	0.177
ε_1	↗	5.185	5.227	5.330	5.871
ε_2	↗	0.439	0.460	0.516	0.862

For $r_d = r_{Sn}$,

$\eta_n \gg 1$	↘	459	183	92	30.5
E_{gn1} in eV	↘	2.863	2.855	2.836	2.735
n	↗	2.152	2.161	2.184	2.302
κ	↗	0.084	0.088	0.098	0.160
ε_1	↗	4.622	4.662	4.760	5.276
ε_2	↗	0.361	0.380	0.429	0.739

x=1

For $r_d = r_{Se}$,

$\eta_n \gg 1$	↘	332	133	66	22
E_{gn1} in eV	↘	2.052	2.046	2.031	1.952
n	↗	3.398	3.404	3.420	3.500
κ	↗	0.977	0.987	1.013	1.154
ε_1	↗	10.591	10.614	10.668	10.920
ε_2	↗	6.640	6.723	6.931	8.076

For $r_d = r_{Te}$,

$\eta_n \gg 1$	↘	331	132.5	66.2	22
E_{gn1} in eV	↘	2.119	2.113	2.098	2.020
n	↗	3.129	3.135	3.151	3.232
κ	↗	0.866	0.875	0.900	1.032
ε_1	↗	9.040	9.063	9.119	9.382
ε_2	↗	5.417	5.489	5.671	6.673

For $r_d = r_{Sn}$,

$\eta_n \gg 1$	↘	331	132	66.2	22
E_{gn1} in eV	↘	2.153	2.147	2.132	2.054
n	↗	2.991	2.997	3.013	3.095
κ	↗	0.812	0.821	0.845	0.974

		20	50	100	300
ε_1	↗	8.286	8.309	8.365	8.631
ε_2	↗	4.858	4.925	5.094	6.027
T in K	↗	20	50	100	300

Table 5p. In the X(x)-system, at E=3.2 eV and $N = 10^{20} \text{cm}^{-3}$, for given r_a and x, and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of $\eta_p (\gg 1, \text{degenerate case})$, 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 $r_a = r_{Ga}$,					
$\eta_p \gg 1$	↘	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 $r_a = r_{In}$,					
$\eta_p \gg 1$	↘	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 $r_a = r_{Cd}$,					
$\eta_p \gg 1$	↘	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 $r_a = r_{Ga}$,					
$\eta_p \gg 1$	↘	395	158	79	26
E_{gp1} in eV	↘	2.848	2.840	2.821	2.719
n	↗	2.590	2.599	2.622	2.741
κ	↗	0.092	0.095	0.106	0.171
ε_1	↗	6.701	6.748	6.866	7.483

		20	50	100	300
ε_2	↗	0.475	0.498	0.559	0.938

For $r_a = r_{In}$,

		20	50	100	300
$\eta_p \gg 1$	↘	369	148	74	25
E_{gp1} in eV	↘	2.823	2.816	2.796	2.695
n	↗	2.530	2.539	2.562	2.680
κ	↗	0.105	0.109	0.121	0.189
ε_1	↗	6.389	6.435	6.550	7.147
ε_2	↗	0.531	0.556	0.619	1.014

For $r_a = r_{Cd}$,

		20	50	100	300
$\eta_p \gg 1$	↘	368.6	147	73.7	24.5
E_{gp1} in eV	↘	2.822	2.815	2.795	2.694
n	↗	2.528	2.537	2.560	2.678
κ	↗	0.105	0.110	0.121	0.190
ε_1	↗	6.381	6.427	6.541	7.138
ε_2	↗	0.534	0.558	0.622	1.018

x=1

For $r_a = r_{Ga}$,

		20	50	100	300
$\eta_p \gg 1$	↘	317	127	63	21
E_{gp1} in eV	↘	2.333	2.327	2.312	2.233
n	↗	3.232	3.239	3.255	3.340
κ	↗	0.557	0.565	0.585	0.693
ε_1	↗	10.137	10.171	10.255	10.673
ε_2	↗	3.605	3.663	3.809	4.628

For $r_a = r_{In}$,

		20	50	100	300
$\eta_p \gg 1$	↘	312	125	62	20.7
E_{gp1} in eV	↘	2.337	2.331	2.316	2.238
n	↗	3.135	3.142	3.158	3.243
κ	↗	0.552	0.560	0.579	0.686
ε_1	↗	9.526	9.559	9.639	10.044
ε_2	↗	3.461	3.517	3.659	4.452

For $r_a = r_{Cd}$,

		20	50	100	300
$\eta_p \gg 1$	↘	311.7	124.6	62	20.7
E_{gp1} in eV	↘	2.337	2.331	2.316	2.2378
n	↗	3.132	3.139	3.155	3.240
κ	↗	0.552	0.559	0.579	0.686
ε_1	↗	9.507	9.539	9.620	10.024
ε_2	↗	3.456	3.513	3.654	4.447

		20	50	100	300
T in K	↗	20	50	100	300