wjert, 2024, Vol. 10 Issue 11, 306-336. Original Article ISSN 2454-695X

World Journal of Engineering Research and Technology
WJERT
www.wjert.org
SJIF Impact Factor: 7.029

OPTICAL COEFFICIENTS IN THE N(P)-TYPE DEGENERATE CdSe(1-x) Te(x)-CRYSTALLINE ALLOY, DUE TO THE NEW STATIC DIELECTRIC CONSTANT-LAW AND THE GENERALIZED MOTT CRITERIUM IN THE METAL-INSULATOR TRANSITION (14)

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.

Article Received on 21/09/2024 **Article Revised on 11/10/2024** **Article Accepted on 01/11/2024**

***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 $\mathbf{CdSe_{1-x}Te_x}$ - crystalline alloy, with $0 \le x \le 1$, 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 $\varepsilon\left(r_{d(a)}, x\right)$-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). 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 $\mathbf{2.88 \times 10^{-7}}$, 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 reported in Tables 1, 2, 3n, 3p, 4n, 4p, 5n, and 5p in Appendix 1.

KEYWORS: $CdSe_{1-x}Te_x$- 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 $\mathbf{X(x) \equiv CdSe_{1-x}Te_x}$ - 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)- crystalline alloy at T=0 K, we denote the donor (acceptor) d(a)-radius by $r_{d(a)}$, and also the intrinsic one by: $r_{do(ao)} = r_{Se(Cd)}$=0.114 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:

$$m_{c(v)}(x)/m_o = 0.095\ (0.82) \times x + 0.11\ (0.45) \times (1 - x). \quad (1)$$

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

$$\varepsilon_o(x) = 10.31 \times x + 10.2 \times (1 - x). \quad (2)$$

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

$$E_{go}(x) = 1.62 \times x + 1.84 \times (1 - x). \quad (3)$$

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

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

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:

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

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

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

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

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

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

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

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 $\varepsilon(r_{d(a)},x) = \frac{\varepsilon_o(x)}{\sqrt{1-\left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3-1\right]\times\ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3}} \geq \varepsilon_o(x)$, with a physical condition: $\left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 < 1$, being a **new $\boldsymbol{\varepsilon(r_{d(a)},x)}$-law**,

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

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. It is interesting to note that, in the p-type case, since $r_a = r_B = 0.088\ \text{nm} \ll r_{ao} = r_{Cd} = 0.148\ \text{nm}$, the above physical condition is not satisfactory as: $\left[\left(\frac{r_B}{r_{Cd}}\right)^3 - 1\right] \times \ln\left(\frac{r_B}{r_{Cd}}\right)^3 = 1.2317701 > 1$. Thus, the B-acceptor can not be taken in the present p-type case.

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:

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

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:

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

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:

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

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 $\boldsymbol{\mathcal{H}_{n(p)} = 0.47137}$, 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 $\mathbf{2.88 \times 10^{-7}}$. Therefore, the density of electrons (holes) given in parabolic conduction (valence) bands can be defined, as that given in compensated materials, by:

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

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:

$$E_{gni(gpi)}(r_{d(a)},x,T) \text{ in eV} = E_{gno(gpo)}(r_{d(a)},x) - 10^{-4} \times T^2 \times \left\{\frac{3.065 \times x}{T+94\text{ K}} + \frac{5.405 \times (1-x)}{T+204\text{ K}}\right\}, \quad (10)$$

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:

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

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:

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

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:

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

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:

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

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

$$\Delta E_{gn}(N, r_d, x) = \Delta E_{gno}(N, r_d, x) \times \{1.8 \times x + 2.2 \times (1 - x)\}, \quad (14n)$$

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

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

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

$$\Delta E_{gp}(N, r_a, x) = \Delta E_{gpo}(N, r_a, x) \times \{50 \times x + 22 \times (1-x)\}, \quad (14p)$$

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

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:

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

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]

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

$$\varepsilon_1 \equiv n^2 - \kappa^2 \text{ and } \varepsilon_2 \equiv 2n\kappa, \quad (16)$$

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, $\varepsilon_{free\ space}$, 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:

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

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 $E \gtrsim E_{gn1(gp1)}$,

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

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

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

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 $n^+(p^+) - p(n)$ $\mathbf{X(x) \equiv CdSe_{1-x}Te_x}$- 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:

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

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

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 $\mathbf{X(x) \equiv CdSe_{1-x}Te_x}$- 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 $\alpha_{MIT}(r_{d(a)}, x) = 0$, 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 $E \to \infty$

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 for T=0K, 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 $\mathbf{X(x) \equiv CdSe_{1-x}Te_x}$ − 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 $\varepsilon(r_{d(a)}, x)$-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).

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 $\mathbf{2.88 \times 10^{-7}}$, 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.

REFERENCES

1. Van Cong, H. Critical density in MIT, obtained in n(p)-type degenerate $InSb_{1-x}P_x(As_x), GaSb_{1-x}P_x(As_x, Te_x), CdSe_{1-x}S_x(Te_x) -$ crystalline alloys, and explained by that of carriers localized in exponential band tails (III). WJERT, 2024; 10(4): 191-220.
2. Van Cong, H. Optical coefficients in the n(p)-type degenerate $CdTe_{1-x}Se_x$- crystalline alloy, due to the new static dielectric constant-law and the generalized Mott criterium in the metal-insulator transition (10). WJERT, 2024; 10(11): 150-178.
3. Van Cong, H. Effects of donor size and heavy doping on optical, electrical and thermoelectric properties of various degenerate donor-silicon systems at low temperatures. American Journal of Modern Physics, 2018; 7: 136-165.
4. Forouhi A. R. & Bloomer I. Optical properties of crystalline semiconductors and dielectrics. Phys. Rev., 1988; 38: 1865-1874.

5. Aspnes, D.E. & Studna, A. A. Dielectric functions and optical parameters of Si, Se, GaP, GaAs, GaSb, InP, InAs, and InSb from 1.5 to 6.0 eV, Phys. Rev. B, 1983; 27: 985-1009.
6. Van Cong, H. et al. Optical bandgap in various impurity-Si systems from the metal-insulator transition study. Physica B, 2014; 436: 130-139.
7. Van Cong, H. et al. Size effect on different impurity levels in semiconductors. Solid State Communications, 1984; 49: 697-699.
8. Van Cong, H. & Debiais, G. A simple accurate expression of the reduced Fermi energy for any reduced carrier density. J. Appl. Phys., 1993; 73: 1545-1546.

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		P	Se	Te	Sn
r_d (nm) [4]	↗	0.110	$\mathbf{r_{do}}$ =**0.114** nm	0.132	0.140
At **x=0**,					
E_{CPE} in meV	↗	1839.84	1840	1843.5	1847.55
n_{MIT}	↘	2.977	2.972	2.874	2.786
$\varepsilon_{1(MIT)}$	↘	8.866	8.836	8.262	7.762
R_{MIT}	↘	0.247	0.246	0.234	0.222
At **x=0.5**,					
E_{CPE} in meV	↗	1729.85	1730	1733.2	1736.96
n_{MIT}	↘	3.051	3.046	2.948	2.859
$\varepsilon_{1(MIT)}$	↘	9.309	9.278	8.689	8.176
R_{MIT}	↘	0.256	0.256	0.243	0.232
At **x=1**,					
E_{CPE} in meV	↗	1619.87	1620	1622.9	1626.38
n_{MIT}	↘	3.124	3.119	3.021	2.933
$\varepsilon_{1(MIT)}$	↘	9.762	9.730	9.126	8.600
R_{MIT}	↘	0.265	0.2647	0.253	0.241

Acceptor		Ga	In	Cd
r_a (nm)	↗	0.126	0.144	$\mathbf{r_{ao}}$**=0.148 nm**
At **x=0**,				
E_{CPE} in meV	↗	1829.1	1839.6	1840
n_{MIT}	↘	3.074	2.976	2.972

$\varepsilon_{1(MIT)}$	↘	9.45	8.85	8.83
R_{MIT}	↘	0.259	0.247	0.246
At **x=0.5**,				
E_{CPE} in meV	↗	1714.8	1729.5	1730
n_{MIT}	↘	3.151	3.049	3.046
$\varepsilon_{1(MIT)}$	↘	9.93	9.30	9.28
R_{MIT}	↘	0.268	0.256	0.2557
At **x=1**,				
E_{CPE} in meV	↗	1600.6	1619.3	1620
n_{MIT}	↘	3.227	3.123	3.119
$\varepsilon_{1(MIT)}$	↘	10.4	9.75	9.73
R_{MIT}	↘	0.277	0.265	0.2647

Table 2. Here, as T=0K and N=$N_{CDn(p)}(r_{d(a)}, x)$, and for $E \to \infty$ 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		P	Se	Te	Sn
At **x=0**,					
n_∞	↘	1.8197	1.8147	1.7187	1.6330
$\varepsilon_{1,\infty}$	↘	3.311	3.293	2.954	2.667
$\sigma_{O,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	8.303	8.281	7.842	7.451
$\propto_\infty$ in $(10^9 \times cm^{-1})$=2.1602					
R_∞	↘	0.084	0.0838	0.0699	0.0578
At **x=0.5**,					
n_∞	↘	1.8246	1.8196	1.7233	1.6374
$\varepsilon_{1,\infty}$	↘	3.329	3.311	2.970	2.681

$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	8.326	8.303	7.864	7.471
$\propto_\infty$ in $(10^9 \times cm^{-1})$= 2.1602					
R_∞	↘	0.085	0.0845	0.0705	0.0584
At **x=1**,					
n_∞	↘	1.8295	1.8245	1.7279	1.6418
$\varepsilon_{1,\infty}$	↘	3.347	3.329	2.986	2.695
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	8.348	8.325	7.885	7.491
$\propto_\infty$ in $(10^9 \times cm^{-1})$= 2.1602					
R_∞	↘	0.086	0.0852	0.0712	0.0590

Acceptor		Ga	In	Cd
		At **x=0**,		
n_∞	↘	1.910	1.818	1.815
$\varepsilon_{1,\infty}$	↘	3.648	3.304	3.293
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	8.715	8.294	8.281
$\propto_\infty$ in $(10^9 \times cm^{-1})$= 2.1602				
R_∞	↘	0.098	0.084	0.0838
At **x=0.5**,				
n_∞	↘	1.915	1.822	1.820
$\varepsilon_{1,\infty}$	↘	3.667	3.322	3.311
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	8.738	8.316	8.303
$\propto_\infty$ in $(10^9 \times cm^{-1})$= 2.1602				
R_∞	↘	0.098	0.0849	0.0845
At **x=1**,				
n_∞	↘	1.920	1.827	1.824
$\varepsilon_{1,\infty}$	↘	3.687	3.340	3.329
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	8.762	8.339	8.325
$\propto_\infty$ in $(10^9 \times cm^{-1})$=2.1602				

R_∞	↘	0.099	0.0856	0.0852

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,		
$\mathbf{E_{CPE} = 1.8398}$	**2.9776**	**0**	**8.8660**	**0**
2	3.087	0.171	9.501	1.055
2.5	3.593	0.165	12.881	1.185
3	3.799	1.106	13.213	8.401
3.5	3.313	1.435	8.915	9.509
4	3.443	1.412	9.859	9.726
4.5	3.750	2.303	8.757	17.269
5	2.322	3.338	−5.753	15.501
5.5	1.272	2.423	−4.253	6.164
6	1.347	1.845	−1.590	4.969
…				
$\mathbf{10^{22}}$	**1.8197**	**0**	**3.3113**	**0**
At x=0.5,				
$\mathbf{E_{CPE}}$ **=1.7298**	**3.0510**	**0**	**9.3088**	**0**
2	3.247	0.202	10.501	1.314
2.5	3.808	0.224	14.454	1.710
3	3.961	1.325	13.933	10.498
3.5	3.359	1.632	8.621	10.961
4	3.493	1.560	9.768	10.898
4.5	3.817	2.497	8.333	19.062
5	2.278	3.575	−7.590	16.285
5.5	1.171	2.571	−5.239	6.019
6	1.262	1.944	−2.185	4.907

…				
10^{22}	**1.8246**	**0**	**3.3292**	**0**
At x=1,				
E_{CPE} =1.6199	**3.1244**	**0**	**9.7622**	**0**
2	3.416	0.217	11.620	1.485
2.5	4.035	0.293	16.198	2.36
3	4.124	1.565	14.562	12.906
3.5	3.399	1.841	8.166	12.513
4	3.538	1.715	9.580	12.135
4.5	3.881	2.699	7.776	20.952
5	2.227	3.819	−9.624	17.014
5.5	1.062	2.723	−6.287	5.785
6	1.172	2.045	−2.809	4.794
…				
10^{22}	**1.8295**	**0**	**3.3470**	**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} =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**
At x=0.5,				
E_{CPE} =1.7148	**3.1508**	**0**	**9.9277**	**0**
2	3.359	0.205	11.242	1.378
2.5	3.928	0.233	15.379	1.834
3	4.073	1.357	14.748	11.052
3.5	3.455	1.659	9.181	11.466
4	3.589	1.581	10.384	11.347
4.5	3.915	2.524	8.959	19.770
5	2.361	3.608	−7.440	17.036
5.5	1.246	2.591	−5.163	6.458
6	1.340	1.957	−2.036	5.246
…				
10^{22}	**1.9150**	**0**	**3.6673**	**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	13.133
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. One notes that, with increasing N, the variations of these optical coefficients depend on those of optical band gap, E_{gn1}.

N (10^{18} cm^{-3})	↗	15	26	60	100
			x=0		
For $\mathbf{r_d} = \mathbf{r_{Se}}$,					
$\eta_n \gg 1$	↗	145	209	366	515
E_{gn1} in eV	↗	1.736	1.748	1.810	1.892
n	↘	3.754	3.742	3.681	3.598
κ	↘	1.589	1.562	1.432	1.267
ε_1	↘	11.567	11.561	11.497	11.343
ε_2	↘	11.931	11.690	10.540	9.121
For $\mathbf{r_d} = \mathbf{r_{Te}}$,					
$\eta_n \gg 1$	↗	144	209	366	515
E_{gn1} in eV	↗	1.763	1.784	1.863	1.961
n	↘	3.631	3.611	3.531	3.433
κ	↘	1.530	1.487	1.324	1.138
ε_1	↘	10.843	10.828	10.718	10.490
ε_2	↘	11.114	10.737	9.353	7.814
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↗	144	208.7	365.7	514.7
E_{gn1} in eV	↗	1.787	1.814	1.909	2.019

n	↘	3.522	3.495	3.400		3.287
κ	↘	1.480	1.423	1.236		1.034
ε_1	↘	10.214	10.188	10.034		9.740
ε_2	↘	10.429	9.950	8.403		6.796

x=0.5

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

$\eta_n \gg 1$	↗	145	209.8	367		516
E_{gn1} in eV	↗	1.616	1.626	1.684		1.762
n	↘	3.875	3.865	3.810		3.733
κ	↘	1.860	1.836	1.704		1.532
ε_1	↗	11.555	11.568	11.609	↘	11.587
ε_2	↘	14.420	14.196	12.988		11.438

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

$\eta_n \gg 1$	↗	144.8	209	367		515.8
E_{gn1} in eV	↗	1.643	1.662	1.737		1.831
n	↘	3.753	3.735	3.661		3.568
κ	↘	1.797	1.754	1.586		1.388
ε_1	↗	10.853	10.871	10.890	↘	10.804
ε_2	↘	13.488	13.105	11.616		9.910

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

$\eta_n \gg 1$	↗	144.5	209		366.5	515.6
E_{gn1} in eV	↗	1.666	1.692		1.783	1.890
n	↘	3.644	3.619		3.531	3.424
κ	↘	1.743	1.686		1.489	1.272
ε_1	↗	10.241	10.258	↘	10.248	10.103
ε_2	↘	12.705	12.203		10.515	8.712

x=1

For $\mathbf{r_d} = \mathbf{r_{Se}}$,					
$\eta_n \gg 1$	↗	150	217	380	535
E_{gn1} in eV	↗	1.506	1.518	1.582	1.667
n	↘	3.984	3.972	3.912	3.831
κ	↘	2.127	2.096	1.941	1.743
ε_1	↗	11.347	11.385	11.539	11.639
ε_2	↘	16.948	16.652	15.189	13.356
For $\mathbf{r_d} = \mathbf{r_{Te}}$,					
$\eta_n \gg 1$	↗	150	217	380	534.8
E_{gn1} in eV	↗	1.533	1.554	1.636	1.736
n	↘	3.862	3.842	3.764	3.667
κ	↘	2.059	2.008	1.814	1.589
ε_1	↗	10.672	10.729	10.880	10.923
ε_2	↘	15.905	15.433	13.659	11.651
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↗	150	217	380	534.7
E_{gn1} in eV	↗	1.557	1.584	1.681	1.795
n	↘	3.753	3.727	3.634	3.523
κ	↘	2.002	1.935	1.710	1.463
ε_1	↗	10.081	10.148	10.284	↘ 10.269
ε_2	↘	15.030	14.402	12.428	10.312
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 $\eta_p (\gg 1$, 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.

One notes that, with increasing N, the variations of these optical coefficients depend on those of optical band gap, E_{gp1}.

$N\ (10^{19}\ cm^{-3})$	↗	6	10	15	20
			x=0		
For $\mathbf{r_a} = \mathbf{r_{Ga}}$,					
$\eta_p \gg 1$	↗	339	492	655	800
E_{gp1} in eV	↗	1.709	1.777	1.869	1.962
n	↘	3.875	3.809	3.717	3.623
κ	↘	1.647	1.501	1.313	1.136
ε_1	↘	12.303	12.253	12.093	11.836
ε_2	↘	12.768	11.434	9.765	8.230
			For $\mathbf{r_a} = \mathbf{r_{In}}$,		
$\eta_p \gg 1$	↗	329	484	648	794
E_{gp1} in eV	↗	1.757	1.838	1.944	2.049
n	↘	3.737	3.656	3.549	3.441
κ	↘	1.544	1.375	1.169	0.982
ε_1	↘	11.577	11.475	11.230	10.879
ε_2	↘	11.542	10.052	8.301	6.759
			For $\mathbf{r_a} = \mathbf{r_{Cd}}$,		
$\eta_p \gg 1$	↗	329	484	648	793.6
E_{gp1} in eV	↗	1.758	1.840	1.946	2.052
n	↘	3.732	3.651	3.544	3.436
κ	↘	1.541	1.371	1.165	0.977
ε_1	↘	11.554	11.450	11.202	10.848
ε_2	↘	11.505	10.011	8.258	6.716
			x=0.5		

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

$\eta_p \gg 1$	↗	288	451	620	768.7
E_{gp1} in eV	↗	1.547	1.606	1.693	1.783
n	↘	4.036	3.980	3.896	3.807
κ	↘	2.025	1.883	1.683	1.487
ε_1	↗	12.186	12.292	12.345 ↘	12.284
ε_2	↘	16.345	14.990	13.117	11.326

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

$\eta_p \gg 1$	↗	258	427	600	750.7
E_{gp1} in eV	↗	1.587	1.658	1.759	1.861
n	↘	3.906	3.838	3.739	3.638
κ	↘	1.929	1.763	1.540	1.329
ε_1	↗	11.533	11.620 ↘	11.612	11.468
ε_2	↘	15.073	13.531	11.518	9.670

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

$\eta_p \gg 1$	↗	256.8	426.5	599	750.05
E_{gp1} in eV	↗	1.588	1.659	1.761	1.863
n	↘	3.902	3.833	3.735	3.633
κ	↘	1.927	1.759	1.536	1.324
ε_1	↗	11.512	11.598 ↘	11.588	11.442
ε_2	↘	15.036	13.489	11.472	9.622

---

x=1

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

$\eta_p \gg 1$	↗	190	385	574	736
E_{gp1} in eV	↗	1.423	1.479	1.577	1.679
n	↘	4.157	4.105	4.013	3.914
κ	↘	2.341	2.195	1.953	1.714

ε_1	↗	11.798	12.030	12.288	12.385
ε_2	↘	19.464	18.019	15.672	13.421

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

$\eta_p \gg 1$	↗	97	327	527	694
E_{gp1} in eV	↗	1.463	1.509	1.619	1.734
n	↘	4.027	3.984	3.879	3.769
κ	↘	2.238	2.120	1.852	1.593
ε_1	↗	11.213	11.380	11.621	11.664
ε_2	↘	18.024	16.890	14.369	12.009

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

$\eta_p \gg 1$	↗	93	324	525	692
E_{gp1} in eV	↗	1.465	1.510	1.620	1.735
n	↘	4.022	3.980	3.875	3.764
κ	↘	2.232	2.118	1.849	1.590
ε_1	↗	11.197	11.358	11.599	11.641
ε_2	↘	17.958	16.861	14.334	11.971

N (10^{19} cm^{-3})	↗	6	10	15	20

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 $\eta_n (\gg 1, \text{degenerate case})$, 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. One notes that, with increasing T, the variations of these optical coefficients depend on those of optical band gap, E_{gn1}.

T in K	↗	20	50	100	300
			x=0		

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

$\eta_n \gg 1$	$\searrow$	515	206	103	34
E_{gn1} in eV	$\searrow$	1.892	1.888	1.876	1.796
n	$\nearrow$	3.598	3.603	3.615	3.694
κ	$\nearrow$	1.267	1.276	1.300	1.460
ε_1	$\nearrow$	11.343	11.353	11.381	11.516
ε_2	$\nearrow$	9.121	9.193	9.402	10.792

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

$\eta_n \gg 1$	$\searrow$	514.9	205.9	103	34.3
E_{gn1} in eV	$\searrow$	1.961	1.957	1.944	1.865
n	$\nearrow$	3.433	3.437	3.450	3.530
κ	$\nearrow$	1.138	1.146	1.169	1.321
ε_1	$\nearrow$	10.490	10.502	10.537	10.716
ε_2	$\nearrow$	7.814	7.879	8.068	9.331

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

$\eta_n \gg 1$	$\searrow$	514.7	205.9	102.9	34.29
E_{gn1} in eV	$\searrow$	2.019	2.015	2.002	1.923
n	$\nearrow$	3.287	3.292	3.305	3.386
κ	$\nearrow$	1.034	1.041	1.063	1.209
ε_1	$\nearrow$	9.740	9.753	9.792	10.003
ε_2	$\nearrow$	6.796	6.856	7.029	8.186

x=0.5

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

$\eta_n \gg 1$	$\searrow$	516	206	103	34.4
E_{gn1} in eV	$\searrow$	1.762	1.758	1.746	1.679
n	$\nearrow$	3.733	3.737	3.748	3.814
κ	$\nearrow$	1.532	1.541	1.566	1.714

ε_1	↗	11.587	11.590	11.598	11.608
ε_2	↗	11.438	11.520	11.740	13.072
For $\mathbf{r_d} = \mathbf{r_{Te}}$,					
$\eta_n \gg 1$	↘	515.8	206	103	34.4
E_{gn1} in eV	↘	1.831	1.827	1.815	1.748
n	↗	3.568	3.572	3.584	3.650
κ	↗	1.388	1.397	1.421	1.562
ε_1	↗	10.804	10.811	10.826	10.885
ε_2	↗	9.910	9.984	10.185	11.402
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↘	515.6	206	103	34.3
E_{gn1} in eV	↘	1.890	1.886	1.874	1.807
n	↗	3.424	3.428	3.440	3.506
κ	↗	1.272	1.281	1.303	1.438
ε_1	↗	10.103	10.111	10.132	10.227
ε_2	↗	8.712	8.781	8.965	10.087
x=1					
For $\mathbf{r_d} = \mathbf{r_{Se}}$,					
$\eta_n \gg 1$	↘	535	214	107	35.6
E_{gn1} in eV	↘	1.667	1.662	1.652	1.597
n	↗	3.831	3.835	3.845	3.898
κ	↗	1.743	1.753	1.777	1.905
ε_1	↘	11.639	11.637	11.630	11.565
ε_2	↗	13.356	13.445	13.665	14.849
For $\mathbf{r_d} = \mathbf{r_{Te}}$,					
$\eta_n \gg 1$	↘	534.8	213.9	106.9	35.6
E_{gn1} in eV	↘	1.736	1.732	1.721	1.666
n	↗	3.667	3.671	3.681	3.735

κ	↗	1.589	1.598	1.621	1.743
ε_1	↗	10.923	10.924	10.926 ↘	10.909
ε_2	↗	11.651	11.732	11.935	13.020

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

$\eta_n \gg 1$	↘	534.7	213.9	106.9	35.6
E_{gn1} in eV	↘	1.795	1.791	1.780	1.725
n	↗	3.522	3.527	3.537	3.591
κ	↗	1.463	1.472	1.494	1.612
ε_1	↗	10.269	10.273	10.281	10.299
ε_2	↗	10.312	10.387	10.574	11.578
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 $\eta_p (\gg 1, \text{degenerate case})$, 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. One notes that, with increasing T, the variations of these optical coefficients depend on those of optical band gap, E_{gp1}.

T in K	↗	20	50	100	300
			x=0		
For $\mathbf{r_a} = \mathbf{r_{Ga}}$,					
$\eta_p \gg 1$	↘	492	197	98	33
E_{gp1} in eV	↘	1.777	1.773	1.760	1.681
n	↗	3.809	3.813	3.825	3.903
κ	↗	1.501	1.510	1.537	1.711
ε_1	↗	12.253	12.258	12.271	12.304
ε_2	↗	11.434	11.517	11.758	13.354

For $\mathbf{r}_a = \mathbf{r}_{In}$,

$\eta_p \gg 1$	$\searrow$	484	194	97	32
E_{gp1} in eV	$\searrow$	1.838	1.834	1.821	1.742
n	$\nearrow$	3.656	3.660	3.673	3.751
κ	$\nearrow$	1.375	1.384	1.409	1.576
ε_1	$\nearrow$	11.475	11.483	11.503	11.586
ε_2	$\nearrow$	10.052	10.128	10.350	11.822

For $\mathbf{r}_a = \mathbf{r}_{Cd}$,

$\eta_p \gg 1$	$\searrow$	484	193.6	96.8	32.2
E_{gp1} in eV	$\searrow$	1.840	1.836	1.823	1.744
n	$\nearrow$	3.651	3.655	3.668	3.746
κ	$\nearrow$	1.371	1.380	1.405	1.572
ε_1	$\nearrow$	11.450	11.458	11.478	11.563
ε_2	$\nearrow$	10.011	10.087	10.3080	11.776

---

x=0.5

For $\mathbf{r}_a = \mathbf{r}_{Ga}$,

$\eta_p \gg 1$	$\searrow$	451	180	90	30
E_{gp1} in eV	$\searrow$	1.606	1.602	1.590	1.523
n	$\nearrow$	3.980	3.984	3.995	4.058
κ	$\nearrow$	1.883	1.893	1.921	2.084
ε_1	$\searrow$	12.292	12.286	12.269	12.126
ε_2	$\nearrow$	14.990	15.087	15.348	16.919

For $\mathbf{r}_a = \mathbf{r}_{In}$,

$\eta_p \gg 1$	$\searrow$	427	171	85	28.5
E_{gp1} in eV	$\searrow$	1.658	1.653	1.642	1.575
n	$\nearrow$	3.838	3.842	3.853	3.917
κ	$\nearrow$	1.763	1.773	1.799	1.958
ε_1	$\searrow$	11.620	11.617	11.607	11.510

ε_2	↗	13.531	13.622	13.866	15.338

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

$\eta_p \gg 1$	↘	426.5	170.6	85	28.4
E_{gp1} in eV	↘	1.659	1.655	1.643	1.576
n	↗	3.833	3.837	3.848	3.913
κ	↗	1.759	1.769	1.796	1.954
ε_1	↘	11.598	11.595	11.586	11.490
ε_2	↗	13.489	13.580	13.823	15.292

x=1

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

$\eta_p \gg 1$	↘	385	154	77	25.7
E_{gp1} in eV	↘	1.479	1.475	1.464	1.409
n	↗	4.105	4.109	4.118	4.169
κ	↗	2.195	2.206	2.233	2.376
ε_1	↘	12.030	12.015	11.975	11.734
ε_2	↗	18.019	18.126	18.392	19.820

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

$\eta_p \gg 1$	↘	327	131	65	21.7
E_{gp1} in eV	↘	1.509	1.505	1.494	1.439
n	↗	3.984	3.988	3.998	4.049
κ	↗	2.120	2.130	2.157	2.298
ε_1	↘	11.380	11.366	11.331	11.112
ε_2	↗	16.890	16.992	17.247	18.615

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

$\eta_p \gg 1$	↘	324	130	65	21.6
E_{gp1} in eV	↘	1.510	1.505	1.495	1.440
n	↗	3.980	3.984	3.994	4.045

κ	↗	2.118	2.129	2.155	2.297
ε_1	↘	11.358	11.345	11.310	11.091
ε_2	↗	16.861	16.963	17.218	18.584
T in K	↗	20	50	100	300