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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)

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ABTRACT

In the n(p)-type $\mathbf{CdTe_{1-x}Se_x}$- 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 $\varepsilon(r_{d(a)}, x)$-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 2.82×10^{-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: $CdTe_{1-x}Se_x$- 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 $\mathbf{X(x) \equiv CdTe_{1-x}Se_x}$ - 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)- crystalline alloy at T=0 K, we denote the donor (acceptor) d(a)-radius by $r_{d(a)}$, and also the intrinsic one by: $r_{do(ao)} = r_{Te(Cd)}$ =0.132 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:

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

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

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

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

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

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:

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

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 $V= (4\pi/3) \times \left(r_{d(a)}\right)^3$, $V_{do(ao)} = (4\pi/3) \times \left(r_{do(ao)}\right)^3$, 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:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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:

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

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:

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

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

Furthermore, by using $\mathbf{M}_{\mathbf{n(p)}} = \mathbf{0.25}$, according to the empirical Heisenberg parameter $\boldsymbol{\mathcal{H}}_{\mathbf{n(p)}} = \mathbf{0.47137}$, 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 2.82×10^{-7}. Therefore, the density of electrons (holes) given in parabolic conduction (valence) bands can be defined, as that given in compensated materials, by:

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

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:

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

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:

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

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:

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

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

$$\Delta E_{gn}(N, r_d, x) = \Delta E_{gno}(N, r_d, x) \times \{1.38 \times x + 2 \times (1 - x)\}, \quad (14n)$$

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:

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

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

$$\Delta E_{gp}(N, r_a, x) = \Delta E_{gpo}(N, r_a, x) \times \{15 \times x + 100 \times (1 - x)\}, \quad (14p)$$

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, $\Delta E_{gn(gp)}\left(N, r_{d(a)}, x\right) = 0$.

OPTICAL BAND GAP

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

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

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: $E_{gn1(gp1)}\left(r_{d(a)}, x\right) = E_{gno(gpo)}\left(r_{d(a)}, x\right)$, 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]

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

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

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:

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

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

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

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

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

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

$$\kappa(E, N, r_{d(a)}, x, T) = G(E) \times E_{gni(gpi)}^{3/2} \times \left(E^* \equiv E - E_{gn1(gp1)}\right)^{1/2}, \text{ for } E_{gni(gpi)} \le E \le 2.3 \text{ eV},$$
$$= F(E) \times \left(E^* \equiv E - E_{gn1(gp1)}\right)^2, \text{ for } E \ge 2.3 \text{ eV}, \quad (20)$$

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 $\mathbf{X(x)} \equiv \mathbf{CdTe_{1-x}Se_x}$- 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 $\alpha_{MIT}(r_{d(a)}, x) = 0$, 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 → ∞

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 $\mathbf{X(x) \equiv CdTe_{1-x}Se_x}$ −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 $\varepsilon(r_{d(a)}, x)$-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 2.82×10^{-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.

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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		P	Te	Sb	Sn
r_d (nm) [4]	↗	0.110	0.132	0.136	0.140
At **x=0**,					
E_{CPE} in meV	↗	1617.2	1620	1620.1	1620.4
n_{MIT}	↘	3.245	3.119	3.115	3.104
$\varepsilon_{1(MIT)}$	↘	10.53	9.73	9.71	9.63
R_{MIT}	↘	0.280	0.265	0.264	0.263
At **x=0.5**,					
E_{CPE} in meV	↗	1726.9	1730	1730.1	1730.4
n_{MIT}	↘	3.113	3.046	3.042	2.977
$\varepsilon_{1(MIT)}$	↘	9.69	9.28	9.25	8.86
R_{MIT}	↘	0.264	0.256	0.255	0.247
At **x=1**,					
E_{CPE} in meV	↗	1836.7	1840	1840.1	1840.5
n_{MIT}	↘	2.980	2.972	2.969	2.848
$\varepsilon_{1(MIT)}$	↘	8.88	8.83	8.81	8.11
R_{MIT}	↘	0.247	0.246	0.246	0.231

Acceptor		Ga	In	Cd
r_a (nm)	↗	0.126	0.144	0.148
At **x=0**,				
E_{CPE} in meV	↗	1600.6	1619.3	1620
n_{MIT}	↘	3.227	3.123	3.119

$\varepsilon_{1(MIT)}$	↘	10.41		9.75		9.73
R_{MIT}	↘	0.277		0.265		0.265
			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		0.2559
			At **x=1**,			
E_{CPE} in meV	↗	1829.1		1839.6		1840
n_{MIT}		2.958	↗	2.976	↘	2.862
$\varepsilon_{1(MIT)}$		8.75	↗	8.85	↘	8.19
R_{MIT}		0.245	↗	0.247	↘	0.232

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	Te	Sb	Sn
			At **x=0**,		
n_{∞}	↘	1.9479	1.8245	1.8207	1.8093
$\varepsilon_{1,\infty}$	↘	3.7945	3.3287	3.3149	3.2734
$\sigma_{O,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	8.8887	8.3253	8.3079	8.2558
α_{∞} in $(10^9 \times cm^{-1})$=		2.1602			
R_{∞}	↘	0.1034	0.0852	0.0846	0.0830
At **x=0.5**,					
n_{∞}	↘	1.8851	1.8196	1.8158	1.7508
$\varepsilon_{1,\infty}$	↘	3.5535	3.3110	3.2972	3.0655
$\sigma_{O,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	8.6017	8.3030	8.2857	7.9892

α_∞ in $(10^9 \times cm^{-1})$= 2.1602					
R_∞	$\searrow$	0.0940	0.0845	0.0839	0.0745
At **x=1**,					
n_∞	$\searrow$	1.8200	1.8147	1.8109	1.6904
$\varepsilon_{1,\infty}$	$\searrow$	3.3124	3.2932	3.2795	2.8575
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	$\searrow$	8.3048	8.2807	8.2634	7.7135
α_∞ in $(10^9 \times cm^{-1})$= 2.1602					
R_∞	$\searrow$	0.0845	0.0838	0.0832	0.0658

Acceptor		Ga		In		Cd
				At **x=0**,		
n_∞	$\searrow$	1.920		1.827		1.824
$\varepsilon_{1,\infty}$	$\searrow$	3.687		3.340		3.329
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	$\searrow$	8.762		8.339		8.325
α_∞ in $(10^9 \times cm^{-1})$= 2.1602						
R_∞	$\searrow$	0.099		0.086		0.085
At **x=0.5**,						
n_∞	$\searrow$	1.915		1.822		1.820
$\varepsilon_{1,\infty}$	$\searrow$	3.667		3.322		3.311
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	$\searrow$	8.738		8.316		8.303
α_∞ in $(10^9 \times cm^{-1})$= 2.1602						
R_∞	$\searrow$	0.098		0.085		0.084
At **x=1**,						
n_∞		1.794	$\nearrow$	1.818	$\searrow$	1.705
$\varepsilon_{1,\infty}$		3.218	$\nearrow$	3.304	$\searrow$	2.906
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$		8.186	$\nearrow$	8.294	$\searrow$	7.778
α_∞ in $(10^9 \times cm^{-1})$= 2.1602						
R_∞		0.081	$\nearrow$	0.084	$\searrow$	0.068

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,		
$\mathbf{E_{CPE} = 1.6172}$	**3.2446**	**0**	**10.5273**	**0**
2	3.538	0.218	12.473	1.540
2.5	4.159	0.295	17.213	2.454
3	4.247	1.571	15.568	13.340
3.5	3.518	1.846	8.972	12.989
4	3.658	1.718	10.426	12.573
4.5	4.001	2.704	8.694	21.639
5	2.344	3.825	−9.135	17.937
5.5	1.178	2.729	−6.048	6.424
6	1.288	2.048	−2.534	5.276
…				
$\mathbf{10^{22}}$	**1.9479**	**0**	**3.7945**	**0**
At x=0.5,				
$\mathbf{E_{CPE}}$ **=1.7269**	**3.1133**	**0**	**9.6927**	**0**
2	3.311	0.203	10.925	1.344
2.5	3.875	0.226	14.962	1.753
3	4.026	1.331	14.434	10.718
3.5	3.420	1.637	9.021	11.199
4	3.555	1.564	10.189	11.118
4.5	3.879	2.502	8.784	19.413
5	2.337	3.581	−7.363	16.737
5.5	1.228	2.575	−5.121	6.325
6	1.320	1.946	−2.045	5.140
…				
$\mathbf{10^{22}}$	**1.8851**	**0**	**3.5535**	**0**

At x=1,				
E_{CPE} =1.8367	**2.9798**	**0**	**8.8795**	**0**
2	3.092	0.172	9.529	1.064
2.5	3.600	0.166	12.925	1.199
3	3.804	1.112	13.236	8.458
3.5	3.314	1.441	8.910	9.549
4	3.445	1.416	9.859	9.759
4.5	3.752	2.308	8.748	17.320
5	2.321	3.345	−5.803	15.525
5.5	1.269	2.427	−4.280	6.161
6	1.344	1.848	−1.607	4.968
…				
10^{22}	**1.8200**	**0**	**3.3124**	**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} = 1.6006	**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**
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} =1.8291	**2.9586**	**0**	**8.7532**	**0**
2	3.076	0.175	9.432	1.076
2.5	3.587	0.170	12.839	1.222
3	3.789	1.126	13.088	8.534
3.5	3.291	1.454	8.720	9.570
4	3.422	1.426	9.675	9.763
4.5	3.730	2.321	8.525	17.318
5	2.291	3.361	−6.045	15.404
5.5	1.236	2.437	−4.412	6.026
6	1.312	1.854	−1.716	4.868
…				
10^{22}	**1.7940**	**0**	**3.2185**	**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 $\mathbf{r_d} = \mathbf{r_{Te}}$,							
$\eta_n \gg 1$	↗	238		344		602	846
E_{gn1} in eV	↗	1.632		1.703		1.910	2.133
n	↘	3.864		3.796		3.591	3.361
κ	↘	1.822		1.662		1.234	0.844
ε_1		11.612	↗	11.649	↘	11.371	10.583
ε_2	↘	14.082		12.615		8.862	5.676
For $\mathbf{r_d} = \mathbf{r_{Sb}}$,							
$\eta_n \gg 1$	↗	238		344		602	846
E_{gn1} in eV	↗	1.633		1.704		1.912	2.136
n	↘	3.859		3.791		3.584	3.354
κ	↘	1.819		1.658		1.229	0.839
ε_1		11.584	↗	11.620	↘	11.337	10.543
ε_2	↘	14.042		12.570		8.813	5.631
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,							
$\eta_n \gg 1$	↗	238		344		602	846
E_{gn1} in eV	↗	1.637		1.709		1.919	2.145
n	↘	3.844		3.774		3.566	3.332
κ	↘	1.811		1.647		1.215	0.825
ε_1		11.500	↗	11.533	↘	11.237	10.425

ε_2	↘	13.922	12.436	8.667	5.496

x=0.5

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

$\eta_n \gg 1$	↗	130	188	329	463
E_{gn1} in eV	↗	1.659	1.676	1.742	1.825
n	↘	3.833	3.817	3.752	3.671
κ	↘	1.759	1.722	1.575	1.402
ε_1	↘	11.598	11.606	11.601	11.511
ε_2	↘	13.487	13.144	11.822	10.292

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

$\eta_n \gg 1$	↗	130	188	329	463
E_{gn1} in eV	↗	1.660	1.677	1.744	1.827
n	↘	3.828	3.812	3.747	3.665
κ	↘	1.757	1.719	1.571	1.397
ε_1	↘	11.569	11.578	11.571	11.4801
ε_2	↘	13.453	13.105	11.774	10.239

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

$\eta_n \gg 1$	↗	128	187	328	462
E_{gn1} in eV	↗	1.778	1.830	1.973	2.120
n	↘	3.649	3.597	3.453	3.301
κ	↘	1.499	1.390	1.116	0.865
ε_1	↘	11.066	11.003	10.677	10.147
ε_2	↘	10.938	10.003	7.707	5.709

x=1

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

$\eta_n \gg 1$	↗	93	135	236	332
E_{gn1} in eV	↗	1.785	1.796	1.841	1.898

n	↘	3.705	3.695	3.650	3.593
κ	↘	1.484	1.462	1.369	1.256
ε_1	↘	11.529	11.517	11.449	11.329
ε_2	↘	10.998	10.801	9.995	9.028

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

$\eta_n \gg 1$	↗	93	135	236	332
E_{gn1} in eV	↗	1.786	1.797	1.843	1.900
n	↘	3.701	3.690	3.645	3.587
κ	↘	1.482	1.460	1.366	1.253
ε_1	↘	11.500	11.487	11.419	11.298
ε_2	↘	10.973	10.773	9.960	8.989

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

$\eta_n \gg 1$	↗	89	131	233	329
E_{gn1} in eV	↗	1.904	1.952	2.076	2.200
n	↘	3.462	3.414	3.286	3.156
κ	↘	1.245	1.154	0.936	0.742
ε_1	↘	10.439	10.321	9.921	9.410
ε_2	↘	8.621	7.882	6.152	4.681

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

N (10^{20} cm^{-3})	↗	1	2	3	4

x=0

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

$\eta_p \gg 1$	↗	610	1164	1606	1994
E_{gp1} in eV	↗	1.072	1.217	1.421	1.639
n	↘	4.469	4.343	4.158	3.953
κ	↘	3.358	2.916	2.356	1.806
ε_1	↗	8.698	10.360	11.790	12.366
ε_2	↘	30.019	25.326	19.510	14.279

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

$\eta_p \gg 1$	↗	517	1098	1551	1944
E_{gp1} in eV	↗	1.155	1.337	1.578	1.827
n	↘	4.305	4.143	3.919	3.676
κ	↘	3.100	2.573	1.951	1.397
ε_1	↗	8.917	10.540	11.554	11.565
ε_2	↘	26.692	21.323	15.294	10.269

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

$\eta_p \gg 1$	↗	513	1096	1548	1942
E_{gp1} in eV	↗	1.157	1.340	1.582	1.833
n	↘	4.299	4.137	3.912	3.669
κ	↘	3.093	2.564	1.940	1.385
ε_1	↗	8.919	10.538	11.540	11.534
ε_2	↘	26.598	21.214	15.180	10.162

x=0.5

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

$\eta_p \gg 1$	↗	405	690	924		1131
E_{gp1} in eV	↘	0.979	0.875	0.847	↗	0.850
n	↗	4.543	4.629	4.652	↘	4.650

κ ↗ 3.656 4.005 4.103 ↘ 4.094

ε_1 ↘ 7.271 5.384 4.804 ↗ 4.858

ε_2 ↗ 33.213 37.081 38.177 ↘ 38.077

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

$\eta_p \gg 1$ ↗ 383 674 910 1119

E_{gp1} in eV 1.081 ↘ 1.011 ↗ 1.012 1.039

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n 4.363 ↗ 4.423 ↘ 4.4227 4.399

κ 3.328 ↗ 3.551 ↘ 3.549 3.460

ε_1 7.966 ↘ 6.954 ↗ 6.963 7.379

ε_2 29.043 ↗ 31.415 ↘ 31.395 30.449

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

$\eta_p \gg 1$ ↗ 382.7 673 909 1118

E_{gp1} in eV 1.084 ↘ 1.015 ↗ 1.017 1.045

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n 4.358 ↗ 4.417 ↘ 4.415 4.391

κ 3.318 ↗ 3.537 ↘ 3.533 3.442

ε_1 7.983 ↘ 6.993 ↗ 7.016 7.438

ε_2 28.917 ↗ 31.248 ↘ 31.197 30.228

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x=1

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

$\eta_p \gg 1$ ↗ 196 426 604 759

E_{gp1} in eV ↗ 1.962 2.232 2.456 2.657

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n ↘ 3.507 3.226 2.981 2.754

κ ↘ 1.136 0.695 0.410 0.218

ε_1 ↘ 11.011 9.921 8.717 7.534

ε_2 ↘ 7.972 4.485 2.445 1.201

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

$\eta_p \gg 1$ ↗ 312 511 677 824

E_{gp1} in eV	↗	1.799	1.921	2.042	2.160
n	↘	3.695	3.573	3.449	3.325
κ	↘	1.456	1.213	0.994	0.801
ε_1	↘	11.535	11.294	10.905	10.414
ε_2	↘	10.758	8.670	6.855	5.330
For $\mathbf{r_a} = \mathbf{r_{Cd}}$,					
$\eta_p \gg 1$	↗	135	387	572	730
E_{gp1} in eV	↗	1.915	2.210	2.446	2.656
n	↘	3.466	3.159	2.902	2.666
κ	↘	1.224	0.727	0.421	0.219
ε_1	↘	10.513	9.454	8.246	7.058
ε_2	↘	8.488	4.592	2.443	1.169
$N\ (10^{20}\ cm^{-3})$	↗	1	2	3	4

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 $\mathbf{r_d} = \mathbf{r_{Te}}$,					
$\eta_n \gg 1$	↘	846	339	169	56
E_{gn1} in eV	↘	2.133	2.128	2.118	2.063
n	↗	3.361	3.365	3.376	3.433
κ	↗	0.844	0.851	0.868	0.958
ε_1	↗	10.583	10.601	10.647	10.871

ε_2	↗	5.676	5.729	5.861	6.576

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

$\eta_n \gg 1$	↘	846	338.6	169	56
E_{gn1} in eV	↘	2.135	2.131	2.121	2.066
n	↗	3.354	3.358	3.369	3.426
κ	↗	0.839	0.846	0.863	0.952
ε_1	↗	10.543	10.562	10.608	10.832
ε_2	↗	5.631	5.683	5.815	6.526

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

$\eta_n \gg 1$	↘	846	338.6	169	56
E_{gn1} in eV	↘	2.145	2.141	2.130	2.076
n	↗	3.332	3.337	3.348	3.405
κ	↗	0.825	0.831	0.848	0.936
ε_1	↗	10.425	10.444	10.490	10.717
ε_2	↗	5.496	5.548	5.677	6.378

x=0.5

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

$\eta_n \gg 1$	↘	463	185	92.6	31
E_{gn1} in eV	↘	1.825	1.820	1.809	1.742
n	↗	3.671	3.675	3.687	3.753
κ	↗	1.402	1.411	1.434	1.576
ε_1	↗	11.511	11.518	11.535	11.601
ε_2	↗	10.292	10.369	10.576	11.829

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

$\eta_n \gg 1$	↘	463	185	92.6	31
E_{gn1} in eV	↘	1.827	1.823	1.811	1.744
n	↗	3.665	3.669	3.681	3.747

κ	↗	1.397	1.406	1.429	1.571
ε_1	↗	11.480	11.487	11.504	11.571
ε_2	↗	10.239	10.315	10.522	11.771

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

$\eta_n \gg 1$	↘	462	185	92.4	31
E_{gn1} in eV	↘	2.120	2.115	2.104	2.037
n	↗	3.301	3.305	3.317	3.387
κ	↗	0.865	0.872	0.890	1.003
ε_1	↗	10.147	10.165	10.212	10.467
ε_2	↗	5.709	5.763	5.908	6.793

x=1

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

$\eta_n \gg 1$	↘	332	132.6	66	22
E_{gn1} in eV	↘	1.898	1.894	1.881	1.802
n	↗	3.593	3.597	3.610	3.689
κ	↗	1.256	1.265	1.289	1.449
ε_1	↗	11.329	11.340	11.368	11.509
ε_2	↗	9.028	9.099	9.308	10.695

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

$\eta_n \gg 1$	↘	332	132.6	66	22
E_{gn1} in eV	↘	1.900	1.896	1.883	1.803
n	↗	3.587	3.591	3.604	3.684
κ	↗	1.253	1.261	1.286	1.446
ε_1	↗	11.298	11.308	11.337	11.479
ε_2	↗	8.989	9.060	9.268	10.652

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

$\eta_n \gg 1$	↘	330	132	66	22

E_{gn1} in eV	↘	2.200	2.195	2.183	2.103
n	↗	3.156	3.160	3.174	3.258
κ	↗	0.742	0.748	0.767	0.892
ε_1	↗	9.410	9.429	9.485	9.818
ε_2	↗	4.681	4.729	4.868	5.809
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 $\mathbf{r_a} = \mathbf{r_{Ga}}$,					
$\eta_p \gg 1$	↘	610	244	122	41
E_{gp1} in eV	↘	1.072	1.067	1.057	1.002
n	↗	4.469	4.473	4.482	4.528
κ	↗	3.358	3.372	3.405	3.581
ε_1	↘	8.698	8.640	8.495	7.684
ε_2	↗	30.019	30.164	30.523	32.433
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↘	517	207	103	34
E_{gp1} in eV	↘	1.155	1.151	1.140	1.085
n	↗	4.305	4.308	4.317	4.365
κ	↗	3.100	3.113	3.145	3.315
ε_1	↘	8.917	8.869	8.747	8.064

ε_2	↗	26.692	26.826	27.160	28.938

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

$\eta_p \gg 1$	↘	513	205	102.7	34
E_{gp1} in eV	↘	1.157	1.153	1.142	1.088
n	↗	4.299	4.303	4.312	4.360
κ	↗	3.093	3.106	3.138	3.307
ε_1	↘	8.919	8.871	8.750	8.070
ε_2	↗	26.598	26.732	27.065	28.839

x=0.5

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

$\eta_p \gg 1$	↘	405	162	81	27
E_{gp1} in eV	↘	0.979	0.975	0.963	0.896
n	↗	4.543	4.546	4.556	4.612
κ	↗	3.656	3.670	3.708	3.934
ε_1	↘	7.271	7.200	7.006	5.791
ε_2	↗	33.213	33.369	33.788	36.288

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

$\eta_p \gg 1$	↘	383	153	77	25
E_{gp1} in eV	↘	1.081	1.077	1.065	0.998
n	↗	4.363	4.367	4.377	4.434
κ	↗	3.328	3.341	3.378	3.594
ε_1	↘	7.966	7.908	7.749	6.747
ε_2	↗	29.043	29.186	29.571	31.874

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

$\eta_p \gg 1$	↘	382.7	153	76.5	25
E_{gp1} in eV	↘	1.084	1.080	1.069	1.001
n	↗	4.358	4.361	4.371	4.429

κ	↗	3.318	3.331	3.368	3.583
ε_1	↘	7.983	7.925	7.768	6.771
ε_2	↗	28.917	29.060	29.444	31.740
			x=1		
For $\mathbf{r_a} = \mathbf{r_{Ga}}$,					
$\eta_p \gg 1$	↘	196	78	39	13
E_{gp1} in eV	↘	1.962	1.957	1.945	1.865
n	↗	3.507	3.512	3.525	3.606
κ	↗	1.136	1.144	1.168	1.322
ε_1	↗	11.011	11.024	11.060	11.254
ε_2	↗	7.972	8.039	8.233	9.533
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↘	312	125	62	21
E_{gp1} in eV	↘	1.799	1.794	1.782	1.702
n	↗	3.695	3.699	3.712	3.790
κ	↗	1.456	1.465	1.491	1.663
ε_1	↗	11.535	11.540	11.554	11.597
ε_2	↗	10.758	10.838	11.070	12.608
For $\mathbf{r_a} = \mathbf{r_{Cd}}$,					
$\eta_p \gg 1$	↘	135	54	27	9
E_{gp1} in eV	↘	1.915	1.910	1.898	1.817
n	↗	3.466	3.470	3.483	3.564
κ	↗	1.224	1.233	1.257	1.418
ε_1	↗	10.513	10.523	10.551	10.691
ε_2	↗	8.488	8.557	8.758	10.109
T in K	↗	20	50	100	300