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OPTICAL COEFFICIENTS IN THE N(P)-TYPE DEGENERATE CdSe(1-x) S(x)-CRYSTALLINE ALLOY, DUE TO THE NEW STATIC DIELECTRIC CONSTANT-LAW AND THE GENERALIZED MOTT CRITERIUM IN THE METAL-INSULATOR TRANSITION (15)

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.

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***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 $\mathbf{CdSe_{1-x}S_x}$- crystalline alloy, with $0 \leq x \leq 1$, basing on our two recent works[1,2], for a given x, and with an increasing $r_{d(a)}$, the optical coefficients have been determined, as functions of the photon energy E, total impurity density N, the donor (acceptor) radius $r_{d(a)}$, concentration x, and temperature T.

Those results have been affected by **(i)** the important new $\varepsilon(r_{d(a)}, x)$-law, developed in Equations (8a, 8b), stating that, for a given x, due to the impurity-size effect, ε decreases (↘) with an increasing (↗) $r_{d(a)}$, and then by **(ii)** the generalized Mott critical d(a)-density defined in the metal-insulator transition (MIT), $N_{CDn(NDp)}(r_{d(a)}, x)$, as observed in Equations (8c, 9a). Furthermore, we also showed that $N_{CDn(NDp)}$ is just the density of carriers localized in exponential band tails, with a precision of the order of $\mathbf{2.88 \times 10^{-7}}$, 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.

KEYWORS: $CdSe_{1-x}S_x$- 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 $\mathbf{X(x) \equiv CdSe_{1-x}S_x}$ - 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:

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

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

$$\varepsilon_o(x) = 9 \times x + 10.2 \times (1 - x). \quad (2)$$

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

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

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

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

and then, the isothermal bulk modulus, by:

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

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

Here, the changes in all the energy-band-structure parameters, expressed in terms of the effective relative dielectric constant $\varepsilon(\mathrm{r_{d(a)}}, \mathrm{x})$, developed as follows.

At $\mathrm{r_{d(a)}} = \mathrm{r_{do(ao)}}$, the needed boundary conditions are found to be, for the impurity-atom volume $\mathrm{V} = (4\pi/3) \times (\mathrm{r_{d(a)}})^3$, $\mathrm{V_{do(ao)}} = (4\pi/3) \times (\mathrm{r_{do(ao)}})^3$, for the pressure p, $\mathrm{p_o} = 0$, 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:

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

Furthermore, we also shown that, as $\mathrm{r_{d(a)}} > \mathrm{r_{do(ao)}}$ ($\mathrm{r_{d(a)}} < \mathrm{r_{do(ao)}}$), the compression (dilatation) gives rise to the increase (the decrease) in the energy gap $\mathrm{E_{gn(gp)}}(\mathrm{r_{d(a)}}, \mathrm{x})$, and the effective donor (acceptor)-ionization energy $\mathrm{E_{d(a)}}(\mathrm{r_{d(a)}}, \mathrm{x})$ in absolute values, obtained in the effective Bohr model, which is represented respectively by: $\pm [\Delta\sigma(\mathrm{r_{d(a)}}, \mathrm{x})]_{n(p)}$,

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

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

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

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** **$\boldsymbol{\varepsilon}(\mathbf{r_{d(a)}},\mathbf{x})$-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 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 $\boldsymbol{\varepsilon}(\mathbf{r_{d(a)}},\mathbf{x})$-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. 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:

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

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

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

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

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

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

Furthermore, by using $\mathbf{M_{n(p)}} = \mathbf{0.25}$, 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 $\mathbf{2.88 \times 10^{-7}}$. Therefore, the density of electrons (holes) given in parabolic conduction (valence) bands can be defined, as that given in compensated materials, by:

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

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:

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

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:

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

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:

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

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:

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

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

$$\Delta E_{gn}(N, r_d, x) = \Delta E_{gno}(N, r_d, x) \times \{3.5 \times x + 2.2 \times (1 - x)\}, \quad (14n)$$

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

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

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

$$\Delta E_{gp}(N, r_a, x) = \Delta E_{gpo}(N, r_a, x) \times \{33 \times x + 22 \times (1 - x)\}, \quad (14p)$$

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

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]

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

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

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

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

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

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

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

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:

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

$Y_i\left(E_{gn1(gp1)}\right) = \frac{A_i}{Q_i} \times \left[\frac{B_i \times (E_{gn1(gp1)}^2 + C_i)}{2} - 2E_{gn1(gp1)} C_i\right]$, $Q_i = \frac{\sqrt{4C_i - B_i^2}}{2}$, 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 $\mathbf{X(x) \equiv CdSe_{1-x}S_x}$- 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: $E_{gn1(gp1)}\left(N^* = 0, r_{d(a)}, x, T = 0\right) = E_{gn1(gp1)}\left(r_{d(a)}, x\right) = E_{gno(gpo)}\left(r_{d(a)}, x\right)$.

Then, in this MIT-case, if $E = E_{gn1(gp1)}\left(r_{d(a)}, x\right) = E_{gno(gpo)}\left(r_{d(a)}, x\right)$, which can be defined as the critical photon energy: $E \equiv E_{CPE}\left(r_{d(a)}, x\right)$, one obtains: $\kappa_{MIT}\left(r_{d(a)}, x\right) = 0$ from Eq. (20), and from Eq. (16): $\varepsilon_{2(MIT)}\left(r_{d(a)}, x\right) = 0$, $\sigma_{O(MIT)}\left(r_{d(a)}, x\right) = 0$ and $\propto_{MIT}\left(r_{d(a)}, x\right) = 0$, and the other functions such as : $n_{MIT}\left(r_{d(a)}, x\right)$ from Eq. (21), and $\varepsilon_{1(MIT)}\left(r_{d(a)}, x\right)$ and $R_{MIT}\left(r_{d(a)}, x\right)$ 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: $n\left(E \to \infty, r_{d(a)}, x, T\right) = n_\infty(r_{d(a)}, x) = \sqrt{\varepsilon(r_{d(a)}, x)} \times \frac{\omega_T}{\omega_L}$, $\omega_T = 5.1 \times 10^{13}\ s^{-1}$ [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 $\mathbf{X(x) \equiv CdSe_{1-x}S_x}$ − 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.

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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	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	↗	2209.75	2210	2215.5	2221.9
n_{MIT}	↘	2.693	2.688	2.591	2.504
$\varepsilon_{1(MIT)}$	↘	7.251	7.224	6.714	6.270
R_{MIT}	↘	0.210	0.209	0.196	0.184
At **x=1**,					
E_{CPE} in meV	↗	2579.64	2580	2588	2597.4
n_{MIT}	↘	2.406	2.401	2.306	2.220
$\varepsilon_{1(MIT)}$	↘	5.790	5.766	5.318	4.927
R_{MIT}	↘	0.170	0.1697	0.1561	0.1435

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	↗	2192.9	2209.4	2210
n_{MIT}	↘	2.791	2.691	2.688
$\varepsilon_{1(MIT)}$	↘	7.79	7.24	7.22
R_{MIT}	↘	0.223	0.210	0.209

At **x=1**,				
E_{CPE} in meV	↗	2555.1	2579.1	2580
n_{MIT}	↘	2.506	2.405	2.401
$\varepsilon_{1(MIT)}$	↘	6.28	5.78	5.766
R_{MIT}	↘	0.184	0.170	0.1697

Table 2. Here, as T=0K and $N=N_{CDn(p)}(r_{d(a)},x)$, and for $E \to \infty$ the numerical results of $n_\infty(r_{d(a)},x)$, $\varepsilon_{1,\infty}(r_{d(a)},x)$, $\sigma_{0,\infty}(r_{d(a)},x)$, $\alpha_\infty(r_{d(a)},x)$ and $R_\infty(r_{d(a)},x)$ go to their appropriate limiting constants.

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
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	8.303	8.281	7.842	7.451
α_∞ in $(10^9 \times cm^{-1})$=2.1602					
R_∞	↘	0.084	0.0838	0.0699	0.0578
At **x=0.5**,					
n_∞	↘	1.7654	1.7605	1.6674	1.5842
$\varepsilon_{1,\infty}$	↘	3.116	3.099	2.780	2.510
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	8.055	8.033	7.608	7.229
α_∞ in $(10^9 \times cm^{-1})$=2.1602					
R_∞	↘	0.077	0.0759	0.0626	0.0511
At **x=1**,					
n_∞	↘	1.7093	1.7046	1.6144	1.5339
$\varepsilon_{1,\infty}$	↘	2.922	2.906	2.606	2.353
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	7.800	7.778	7.367	6.999
α_∞ in $(10^9 \times cm^{-1})$=2.1602					
R_∞	↘	0.068	0.0679	0.0552	0.0444

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_∞ ↘	1.853	1.763	1.760
$\varepsilon_{1,\infty}$ ↘	3.433	3.110	3.099
$\sigma_{O,\infty}$ in $\frac{10^5}{\Omega \times cm}$ ↘	8.455	8.046	8.033
$\propto_\infty$ in $(10^9 \times cm^{-1})$=2.1602			
R_∞ ↘	0.089	0.0763	0.0759

At **x=1**,

n_∞ ↘	1.794	1.707	1.705
$\varepsilon_{1,\infty}$ ↘	3.218	2.915	2.906
$\sigma_{O,\infty}$ in $\frac{10^5}{\Omega \times cm}$ ↘	8.186	7.791	7.778
$\propto_\infty$ in $(10^9 \times cm^{-1})$=2.1602			
R_∞ ↘	0.0808	0.0683	0.0679

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

E in eV	n	κ	ε_1	ε_2
		At x=0,		
$E_{CPE} = 1.8398$	**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
…				
10^{22}	**1.8197**	**0**	**3.3113**	**0**
		At x=0.5,		
E_{CPE} =2.2097	**2.6927**	**0**	**7.2509**	**0**
2.5	2.913	0.032	8.485	0.186

3	3.231	0.513	10.177	3.315
3.5	3.074	0.867	8.700	5.330
4	3.203	0.970	9.321	6.215
4.5	3.463	1.707	9.082	11.821
5	2.385	2.602	−1.085	12.414
5.5	1.522	1.958	−1.519	5.960
6	1.549	1.531	0.054	4.744
…				
10^{22}	**1.7654**	**0**	**3.1165**	**0**
		At x=1,		
E_{CPE} =2.5796	**2.4062**	**0**	**5.7899**	**0**
3	2.681	0.145	7.167	0.778
3.5	2.765	0.441	7.450	2.439
4	2.910	0.610	8.098	3.555
4.5	3.141	1.200	8.428	7.539
5	2.374	1.958	1.804	9.300
5.5	1.688	1.542	0.470	5.208
6	1.683	1.247	1.276	4.197
…				
10^{22}	**1.7093**	**0**	**2.9217**	**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} =2.1929	**2.7907**	**0**	**7.7881**	**0**
2.5	3.026	0.036	9.156	0.216
3	3.341	0.535	10.879	3.576
3.5	3.172	0.889	9.269	5.643
4	3.300	0.988	9.916	6.525
4.5	3.562	1.732	9.689	12.340
5	2.469	2.634	−0.843	13.005
5.5	1.597	1.978	−1.362	6.318
6	1.626	1.545	0.257	5.025
…				
10^{22}	**1.8528**	**0**	**3.4331**	**0**
		At x=1,		
E_{CPE} =2.5551	**2.5062**	**0**	**6.2010**	**0**
3	2.798	0.162	7.802	0.910
3.5	2.868	0.465	8.012	2.667
4	3.012	0.632	8.676	3.807
4.5	3.245	1.231	9.013	7.988
5	2.458	1.998	2.052	9.824
5.5	1.761	1.568	0.639	5.523
6	1.757	1.265	1.486	4.445
…				
10^{22}	**1.7940**	**0**	**3.2185**	**0**
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 $\mathbf{r_d} = \mathbf{r_{Se}}$,

$\eta_n \gg 1$	↗	102	149	262	369
E_{gn1} in eV	↗	2.115	2.121	2.160	2.214
n	↘	3.315	3.309	3.269	3.210
κ	↘	0.872	0.863	0.802	0.720
ε_1	↘	10.229	10.206	10.040	9.789
ε_2	↘	5.780	5.710	5.245	4.625

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

$\eta_n \gg 1$	↗	101.6	148.3	261.3	368.2
E_{gn1} in eV	↗	2.137	2.148	2.199	2.265
n	↘	3.199	3.187	3.133	3.063
κ	↘	0.837	0.820	0.742	0.648
ε_1	↘	9.533	9.487	9.266	8.963
ε_2	↘	5.359	5.225	4.651	3.971

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

$\eta_n \gg 1$	↗	100.6	147.5	260.6	367.7
E_{gn1} in eV	↗	2.156	2.172	2.234	2.308
n	↘	3.096	3.079	3.013	2.933
κ	↘	0.807	0.783	0.692	0.589

ε_1	↘	8.932	8.866	8.601	8.255
ε_2	↘	4.999	4.819	4.169	3.455
			x=1		
For $\mathbf{r_d = r_{Se}}$,					
$\eta_n \gg 1$	↗	77.32	114	202.5	286
E_{gn1} in eV	↗	2.495	2.497	2.524	2.565
n	↘	2.848	2.846	2.815	2.769
κ	↘	0.367	0.366	0.338	0.298
ε_1	↘	7.978	7.964	7.811	7.579
ε_2	↘	2.101	2.084	1.905	1.654
For $\mathbf{r_d = r_{Te}}$,					
$\eta_n \gg 1$	↗	75.7	112.7	201.5	285.3
E_{gn1} in eV	↗	2.514	2.521	2.557	2.606
n	↘	2.737	2.729	2.688	2.632
κ	↘	0.349	0.342	0.306	0.261
ε_1	↘	7.368	7.332	7.131	6.860
ε_2	↘	1.909	1.867	1.646	1.375
For $\mathbf{r_d = r_{Sn}}$,					
$\eta_n \gg 1$	↗	73.7	111	200.3	284.2
E_{gn1} in eV	↗	2.532	2.542	2.587	2.643
n	↘	2.636	2.624	2.574	2.510
κ	↘	0.331	0.321	0.279	0.230
ε_1	↘	6.839	6.785	6.549	6.249
ε_2	↘	1.744	1.684	1.435	1.155
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^{19} cm^{-3})	↗	8	10	15	20
			x=0		

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

$\eta_p \gg 1$	↗	419	492	655	800
E_{gp1} in eV	↗	1.742	1.777	1.869	1.962
n	↘	3.843	3.809	3.717	3.623
κ	↘	1.576	1.501	1.313	1.136
ε_1	↘	12.287	12.253	12.093	11.836
ε_2	↘	12.114	11.434	9.765	8.230

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

$\eta_p \gg 1$	↗	410	484	648	794
E_{gp1} in eV	↗	1.796	1.838	1.944	2.049
n	↘	3.697	3.656	3.549	3.441
κ	↘	1.460	1.375	1.169	0.982
ε_1	↘	11.537	11.475	11.230	10.879
ε_2	↘	10.796	10.052	8.301	6.759

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

$\eta_p \gg 1$	↗	410	484	648	793.6
E_{gp1} in eV	↗	1.798	1.840	1.946	2.052
n	↘	3.692	3.651	3.544	3.436
κ	↘	1.456	1.371	1.165	0.977
ε_1	↘	11.513	11.450	11.202	10.848
ε_2	↘	10.757	10.011	8.258	6.716

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x=0.5

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

$\eta_p \gg 1$	↗	259	315	437	544
E_{gp1} in eV	↗	2.086	2.108	2.171	2.236
n	↘	3.438	3.415	3.349	3.280
κ	↘	0.920	0.883	0.785	0.689
ε_1	↘	10.975	10.880	10.600	10.283
ε_2	↘	6.327	6.033	5.261	4.521

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

$\eta_p \gg 1$	↗	237	295	420	529
E_{gp1} in eV	↗	2.122	2.148	2.221	2.294
n	↘	3.311	3.283	3.207	3.128

κ	↘	0.862	0.819		0.711	0.608
ε_1	↘	10.222	10.107		9.778	9.413
ε_2	↘	5.706	5.381		4.561	3.806
For $\mathbf{r_a} = \mathbf{r_{Cd}}$,						
$\eta_p \gg 1$	↗	236	294		420	528.6
E_{gp1} in eV	↗	2.123	2.150		2.222	2.296
n	↘	3.307	3.279		3.202	3.123
κ	↘	0.860	0.818		0.709	0.606
ε_1	↘	10.198	10.083		9.752	9.386
ε_2	↘	5.688	5.362		4.540	3.785
=1						
For $\mathbf{r_a} = \mathbf{r_{Ga}}$,						
$\eta_p \gg 1$	↗	116	171		279	370
E_{gp1} in eV	↗	2.437	2.446		2.488	2.536
n	↘	3.002	2.992		2.946	2.891
κ	↘	0.432	0.422		0.376	0.326
ε_1	↘	8.828	8.776		8.536	8.251
ε_2	↘	2.594	2.524		2.216	1.887
For $\mathbf{r_a} = \mathbf{r_{In}}$,						
$\eta_p \gg 1$	↗	48	119		241	337
E_{gp1} in eV	↘	2.480	2.474	↗	2.519	2.574
n	↗	2.868	2.874	↘	2.824	2.762
κ	↗	0.385	0.390	↘	0.344	0.291
ε_1	↗	8.078	8.108	↘	7.859	7.547
ε_2	↗	2.207	2.244	↘	1.944	1.607
For $\mathbf{r_a} = \mathbf{r_{Cd}}$,						
$\eta_p \gg 1$	↗	44	117		240	336.2
E_{gp1} in eV	↘	2.482	2.475	↗	2.519	2.575
n	↗	2.862	2.870	↘	2.821	2.758
κ	↗	0.382	0.389	↘	0.343	0.290
ε_1	↗	8.047	8.087	↘	7.839	7.525
ε_2	↗	2.186	2.235	↘	1.937	1.599
N (10^{19} cm^{-3})	↗	8	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 $\mathbf{r_d = r_{Se}}$,					
$\eta_n \gg 1$	↘	515	206	103	34
E_{gn1} in eV	↘	1.892	1.888	1.876	1.796
n	↗	3.598	3.603	3.615	3.694
κ	↗	1.267	1.276	1.300	1.460
ε_1	↗	11.343	11.353	11.381	11.516
ε_2	↗	9.121	9.193	9.402	10.792
For $\mathbf{r_d = r_{Te}}$,					
$\eta_n \gg 1$	↘	514.9	205.9	103	34.3
E_{gn1} in eV	↘	1.961	1.957	1.944	1.865
n	↗	3.433	3.437	3.450	3.530
κ	↗	1.138	1.146	1.169	1.321
ε_1	↗	10.490	10.502	10.537	10.716
ε_2	↗	7.814	7.879	8.068	9.331
For $\mathbf{r_d = r_{Sn}}$,					
$\eta_n \gg 1$	↘	514.7	205.9	102.9	34.29
E_{gn1} in eV	↘	2.019	2.015	2.002	1.923
n	↗	3.287	3.292	3.305	3.386
κ	↗	1.034	1.041	1.063	1.209
ε_1	↗	9.740	9.753	9.792	10.003
ε_2	↗	6.796	6.856	7.029	8.186
x=0.5					
For $\mathbf{r_d = r_{Se}}$,					
$\eta_n \gg 1$	↘	369	147	74	24.5
E_{gn1} in eV	↘	2.265	2.210	2.198	2.131
n	↗	3.063	3.215	3.227	3.298
κ	↗	0.648	0.726	0.743	0.867

ε_1	↗	8.963	9.809	9.863	10.163
ε_2	↗	3.971	4.672	4.800	5.586
For $\mathbf{r_d} = \mathbf{r_{Te}}$,					
$\eta_n \gg 1$	↘	368.2	147	73.6	24.5
E_{gn1} in eV	↘	2.265	2.261	2.249	2.182
n	↗	3.063	3.068	3.080	3.152
κ	↗	0.648	0.654	0.670	0.768
ε_1	↗	8.963	8.984	9.038	9.344
ε_2	↗	3.971	4.014	4.130	4.845
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↘	368.2	147	73.6	24.5
E_{gn1} in eV	↘	2.265	2.261	2.249	2.182
n	↗	3.062	3.068	3.080	3.152
κ	↗	0.648	0.654	0.670	0.768
ε_1	↗	8.963	8.984	9.038	9.344
ε_2	↗	3.971	4.014	4.130	4.845
			x=1		
For $\mathbf{r_d} = \mathbf{r_{Se}}$,					
$\eta_n \gg 1$	↘	286	114	57	19
E_{gn1} in eV	↘	2.565	2.561	2.550	2.495
n	↗	2.769	2.774	2.786	2.848
κ	↗	0.298	0.303	0.313	0.368
ε_1	↗	7.579	7.603	7.663	7.975
ε_2	↗	1.654	1.679	1.742	2.097
For $\mathbf{r_d} = \mathbf{r_{Te}}$,					
$\eta_n \gg 1$	↘	285.3	114	57	19
E_{gn1} in eV	↘	2.606	2.602	2.592	2.536
n	↗	2.632	2.637	2.649	2.711
κ	↗	0.261	0.265	0.274	0.326
ε_1	↗	6.860	6.884	6.942	7.246
ε_2	↗	1.375	1.397	1.453	1.770
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↘	284.2	113.7	56.8	19

E_{gn1} in eV	↘	2.643	2.638	2.628	2.573
n	↗	2.510	2.515	2.527	2.590
κ	↗	0.230	0.234	0.242	0.292
ε_1	↗	6.249	6.272	6.328	6.623
ε_2	↗	1.155	1.176	1.226	1.511
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 η_p ($\gg 1$, degenerate case), E_{gp1}, n, κ, ε_1 and ε_2, obtained as functions of T, being represented by the arrows: ↗ and ↘, noting that both η_p and E_{gp1} decrease with increasing T. 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 $r_a = r_{Ga}$,					
$\eta_p \gg 1$	↘	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 $r_a = r_{In}$,					
$\eta_p \gg 1$	↘	484	194	97	32
E_{gp1} in eV	↘	1.838	1.834	1.821	1.742
n	↗	3.656	3.660	3.673	3.751
κ	↗	1.375	1.384	1.409	1.576
ε_1	↗	11.475	11.483	11.503	11.586
ε_2	↗	10.052	10.128	10.350	11.822
For $r_a = r_{Cd}$,					
$\eta_p \gg 1$	↘	484	193.6	96.8	32.2
E_{gp1} in eV	↘	1.840	1.836	1.823	1.744
n	↗	3.651	3.655	3.668	3.746
κ	↗	1.371	1.380	1.405	1.572
ε_1	↗	11.450	11.458	11.478	11.563

ε_2	↗	10.011	10.087	10.3080	11.776

x=0.5

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

$\eta_p \gg 1$	↘	315	126	63	21
E_{gp1} in eV	↘	2.108	2.104	2.092	2.025
n	↗	3.415	3.419	3.431	3.501
κ	↗	0.883	0.890	0.909	1.023
ε_1	↗	10.880	10.899	10.948	11.212
ε_2	↗	6.033	6.089	6.240	7.165

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

$\eta_p \gg 1$	↘	295	118	59	20
E_{gp1} in eV	↘	2.148	2.144	2.133	2.065
n	↗	3.283	3.288	3.300	3.370
κ	↗	0.819	0.826	0.844	0.954
ε_1	↗	10.107	10.126	10.176	10.448
ε_2	↗	5.381	5.433	5.573	6.435

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

$\eta_p \gg 1$	↘	294	117.6	58.8	19.6
E_{gp1} in eV	↘	2.150	2.145	2.134	2.066
n	↗	3.279	3.284	3.296	3.366
κ	↗	0.818	0.824	0.842	0.952
ε_1	↗	10.083	10.102	10.152	10.424
ε_2	↗	5.362	5.411	5.554	6.413

x=1

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

$\eta_p \gg 1$	↘	171	68	34	11
E_{gp1} in eV	↘	2.446	2.441	2.431	2.375
n	↗	2.992	2.997	3.009	3.070
κ	↗	0.422	0.426	0.438	0.506
ε_1	↗	8.776	8.801	8.861	9.173
ε_2	↗	2.524	2.556	2.639	3.099

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

$\eta_p \gg 1$	↘	119	48	24	8

E_{gp1} in eV	↘	2.474	2.470	2.459	2.403
n	↗	2.874	2.879	2.891	2.953
κ	↗	0.390	0.395	0.407	0.471
ε_1	↗	8.108	8.132	8.191	8.500
ε_2	↗	2.244	2.275	2.351	2.784
For $\mathbf{r_a} = \mathbf{r_{Cd}}$,					
$\eta_p \gg 1$	↘	117	47	23	7.72
E_{gp1} in eV	↘	2.475	2.471	2.460	2.403
n	↗	2.871	2.875	2.887	2.950
κ	↗	0.389	0.394	0.406	0.470
ε_1	↗	8.087	8.111	8.170	8.479
ε_2	↗	2.235	2.266	2.343	2.774
T in K	↗	20	50	100	300