



**OPTICAL COEFFICIENTS IN THE N(P)-TYPE DEGENERATE
GaSb(1-x) Te(x)-CRYSTALLINE ALLOY, DUE TO THE NEW STATIC
DIELECTRIC CONSTANT-LAW AND THE GENERALIZED MOTT
CRITERIUM IN THE METAL-INSULATOR TRANSITION (13)**

Pr. Dr. Huynh Van Cong* and Pr. Dr. Paul Blaise

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**

Pr. 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.

ABSTRACT

In the n(p)-type $\text{GaSb}_{1-x}\text{Te}_x$ - crystalline alloy, with $0 \leq x \leq 1$, basing on our two recent works^[1,2], for a given x, and with an increasing $r_{d(a)}$, the optical coefficients have been determined, as functions of the photon energy E, total impurity density N, the donor (acceptor) radius $r_{d(a)}$, concentration x, and temperature T. Those results have been affected by (i) the important new $\epsilon(r_{d(a)}, x)$ -law, developed in Equations (8a, 8b), stating that, for a given x, due to the impurity-size effect, ϵ decreases (\searrow) with an increasing (\nearrow) $r_{d(a)}$, and then by (ii) the generalized Mott critical d(a)-density defined in the metal-insulator transition (MIT), $N_{CDn(NDp)}(r_{d(a)}, x)$, as observed in

Equations (8c, 9a). Furthermore, we also showed that $N_{CDn(NDp)}$ is just the density of carriers localized in exponential band tails, with a precision of the order of 2.87×10^{-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 $\epsilon(r_{d(a)}, x)$ -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.

KEYWORDS: GaSb_{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 $\mathbf{X(x)} \equiv \text{GaSb}_{1-x}\text{Te}_x$ - 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 STRUCTURE 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: $r_{do(ao)} = r_{Sb(Ga)} = 0.136$ nm (0.126 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:

$$m_{c(v)}(x)/m_o = 0.209 (0.4) \times x + 0.047 (0.3) \times (1 - x). \quad (1)$$

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

$$\epsilon_o(x) = 12.3 \times x + 15.69 \times (1 - x). \quad (2)$$

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

$$E_{go}(x) = 1.796 \times x + 0.81 \times (1 - x). \quad (3)$$

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

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

and then, the isothermal bulk modulus, by:

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

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

Here, the changes in all the energy-band-structure parameters, expressed in terms of the effective relative dielectric constant $\epsilon(r_{d(a)}, x)$, 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:

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

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

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

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

$$E_{\text{gno(gp0)}}(r_{\text{d(a)}}, x) - E_{\text{go}}(x) = E_{\text{d(a)}}(r_{\text{d(a)}}, x) - E_{\text{do(ao)}}(x) = E_{\text{do(ao)}}(x) \times \left[\left(\frac{\epsilon_0(x)}{\epsilon(r_{\text{d(a)}})} \right)^2 - 1 \right] = - [\Delta\sigma(r_{\text{d(a)}}, x)]_{\text{n(p)}} \quad (7)$$

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

(i)-for $r_{\text{d(a)}} \geq r_{\text{do(ao)}}$, since $\epsilon(r_{\text{d(a)}}, x) = \frac{\epsilon_0(x)}{\sqrt{1 + \left[\left(\frac{r_{\text{d(a)}}}{r_{\text{do(ao)}}} \right)^3 - 1 \right] \times \ln \left(\frac{r_{\text{d(a)}}}{r_{\text{do(ao)}}} \right)^3}} \leq \epsilon_0(x)$, being a **new**

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

$$E_{\text{gno(gp0)}}(r_{\text{d(a)}}, x) - E_{\text{go}}(x) = E_{\text{d(a)}}(r_{\text{d(a)}}, x) - E_{\text{do(ao)}}(x) = E_{\text{do(ao)}}(x) \times \left[\left(\frac{r_{\text{d(a)}}}{r_{\text{do(ao)}}} \right)^3 - 1 \right] \times \ln \left(\frac{r_{\text{d(a)}}}{r_{\text{do(ao)}}} \right)^3 \geq 0, \quad (8a)$$

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

(ii)-for $r_{\text{d(a)}} \leq r_{\text{do(ao)}}$, since $\epsilon(r_{\text{d(a)}}, x) = \frac{\epsilon_0(x)}{\sqrt{1 - \left[\left(\frac{r_{\text{d(a)}}}{r_{\text{do(ao)}}} \right)^3 - 1 \right] \times \ln \left(\frac{r_{\text{d(a)}}}{r_{\text{do(ao)}}} \right)^3}} \geq \epsilon_0(x)$, with a

condition, given by: $\left[\left(\frac{r_{\text{d(a)}}}{r_{\text{do(ao)}}} \right)^3 - 1 \right] \times \ln \left(\frac{r_{\text{d(a)}}}{r_{\text{do(ao)}}} \right)^3 < 1$, being a **new** $\epsilon(r_{\text{d(a)}}, x)$ -law,

$$E_{\text{gno(gp0)}}(r_{\text{d(a)}}, x) - E_{\text{go}}(x) = E_{\text{d(a)}}(r_{\text{d(a)}}, x) - E_{\text{do(ao)}}(x) = -E_{\text{do(ao)}}(x) \times \left[\left(\frac{r_{\text{d(a)}}}{r_{\text{do(ao)}}} \right)^3 - 1 \right] \times \ln \left(\frac{r_{\text{d(a)}}}{r_{\text{do(ao)}}} \right)^3 \leq 0, \quad (8b)$$

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

$$a_{\text{Bn(Bp)}}(r_{\text{d(a)}}, x) \equiv \frac{\epsilon(r_{\text{d(a)}}, x) \times \hbar^2}{m_{\text{c(v)}}(x) \times q^2} = 0.53 \times 10^{-8} \text{ cm} \times \frac{\epsilon(r_{\text{d(a)}}, x)}{m_{\text{c(v)}}(x)/m_0}. \quad (8c)$$

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

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

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

$$r_{sn(sp)}(N, r_{d(a)}, x) \equiv \left(\frac{3}{4\pi N}\right)^{1/3} \times \frac{1}{a_{Bn(Bp)}(r_{d(a)}, x)} = 1.1723 \times 10^8 \times \left(\frac{1}{N}\right)^{1/3} \times \frac{m_{c(v)}(x)/m_0}{\varepsilon(r_{d(a)}, x)}, \quad (9b)$$

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:

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

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

Furthermore, by using $M_{n(p)} = 0.25$, according to the empirical Heisenberg parameter $\mathcal{H}_{n(p)} = 0.47137$, as those given in Equations (8, 15) of the Ref.^[1], we have also showed that $N_{CDn(CDp)}$ is just the density of electrons (holes) localized in the exponential conduction (valence)-band tail, with a precision of the order of 2.87×10^{-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 $E_{g_{ni}(gpi)}(r_{d(a)}, x, T)$ at any T is given by:

$$E_{g_{ni}(gpi)}(r_{d(a)}, x, T) \text{ in eV} = E_{g_{no}(gpo)}(r_{d(a)}, x) - 10^{-4} \times T^2 \times \left\{ \frac{5.405 \times x}{T+204 \text{ K}} + \frac{3.065 \times (1-x)}{T+94 \text{ K}} \right\}, \quad (10)$$

suggesting that, for given x and $r_{d(a)}$, $E_{g_{ni}(gpi)}$ 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:

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

where $m_r(x)/m_0$ is the reduced effective mass $m_r(x)/m_0$, 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 η_{n(p)} or the Fermi energy E_{Fn}(-E_{Fp}), obtained for any T and any effective d(a)-density, N*(N, r_{d(a)}, x) = N*, defined in Eq. (9d), for a simplicity of presentation, being investigated in our previous paper^[8], with a precision of the order of 2.11 × 10⁻⁴, is found to be given by:

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

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

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

and $G(u) \simeq \text{Ln}(u) + 2^{-\frac{3}{2}} \times u \times e^{-du}$; $d = 2^{3/2} \left[\frac{1}{\sqrt{27}} - \frac{3}{16} \right] > 0$. 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:

$$\Delta E_{\text{gno}}(N, r_d, x) = a_1 \times \frac{\varepsilon_0(x)}{\varepsilon(r_d, x)} \times N_r^{1/3} + a_2 \times \frac{\varepsilon_0(x)}{\varepsilon(r_d, x)} \times N_r^{1/3} \times (2.503 \times [-E_{\text{cn}}(r_{\text{sn}}) \times r_{\text{sn}}]) + a_3 \times \left[\frac{\varepsilon_0(x)}{\varepsilon(r_d, x)} \right]^{5/4} \times \sqrt{\frac{m_v}{m_r}} \times N_r^{1/4} + a_4 \times \sqrt{\frac{\varepsilon_0(x)}{\varepsilon(r_d, x)}} \times N_r^{1/2} \times 2 + a_5 \times \left[\frac{\varepsilon_0(x)}{\varepsilon(r_d, x)} \right]^{3/2} \times N_r^{1/6}$$

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

$$\Delta E_{\text{gn}}(N, r_d, x) = \Delta E_{\text{gno}}(N, r_d, x) \times \{1.9 \times x + 0.7 \times (1 - x)\}, \tag{14n}$$

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

$$\Delta E_{\text{gpo}}(N, r_a, x) = a_1 \times \frac{\varepsilon_0(x)}{\varepsilon(r_a, x)} \times N_r^{1/3} + a_2 \times \frac{\varepsilon_0(x)}{\varepsilon(r_a, x)} \times N_r^{1/3} \times (2.503 \times [-E_{\text{cp}}(r_{\text{sp}}) \times r_{\text{sp}}]) + a_3 \times \left[\frac{\varepsilon_0(x)}{\varepsilon(r_a, x)} \right]^{5/4} \times \sqrt{\frac{m_c}{m_r}} \times N_r^{1/4} + 2a_4 \times \sqrt{\frac{\varepsilon_0(x)}{\varepsilon(r_a, x)}} \times N_r^{1/2} + a_5 \times \left[\frac{\varepsilon_0(x)}{\varepsilon(r_a, x)} \right]^{3/2} \times N_r^{1/6}$$

$$N_r \equiv \left(\frac{N^*}{N_{\text{CDp}}(r_a, x)} \right), \Delta E_{\text{gp}}(N, r_a, x) = \Delta E_{\text{gpo}}(N, r_a, x) \times \{8 \times x + 12 \times (1 - x)\}, \tag{14p}$$

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

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

OPTICAL BAND GAP

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

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

where $E_{\text{gin(gp)}}, [+E_{\text{Fn}}, -E_{\text{Fp}}] \geq 0$, and $\Delta E_{\text{gn(gp)}}$ are respectively determined in Equations [10, 12, 14n(p)], respectively. So, as noted above, at the MIT, Eq. (15) thus becomes: $E_{\text{gn1(gp1)}}(r_{\text{d(a)}, \mathbf{x}}) = E_{\text{gn0(gp0)}}(r_{\text{d(a)}, \mathbf{x}}$, according to: $N = N_{\text{CDn(NDp)}}(r_{\text{d(a)}, \mathbf{x}}$.

OPTICAL COEFFICIENTS

The optical properties of any medium can be described by the complex refraction index \mathbf{N} and the complex dielectric function ϵ , $\mathbf{N} \equiv \mathbf{n} - i\kappa$ and $\epsilon \equiv \epsilon_1 - i\epsilon_2$, where $i^2 = -1$ and $\epsilon \equiv \mathbf{N}^2$. 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 \mathbf{n} and the extinction coefficient κ as: $\epsilon_1 \equiv \mathbf{n}^2 - \kappa^2$ and $\epsilon_2 \equiv 2\mathbf{n}\kappa$. One notes that the optical absorption coefficient α is related to ϵ_2 , \mathbf{n} , κ , and the optical conductivity σ_0 , by^[2]

$$\alpha(E, \mathbf{N}, r_{\text{d(a)}, \mathbf{x}}, T) \equiv \frac{\hbar q^2 \times |v(E)|^2}{n(E) \times \epsilon_{\text{free space}} \times c E} \times J(E^*) = \frac{E \times \epsilon_2(E)}{\hbar c n(E)} \equiv \frac{2E \times \kappa(E)}{\hbar c} \equiv \frac{4\pi \sigma_0(E)}{c n(E) \times \epsilon_{\text{free space}}},$$

$$\epsilon_1 \equiv \mathbf{n}^2 - \kappa^2 \text{ and } \epsilon_2 \equiv 2\mathbf{n}\kappa, \tag{16}$$

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

Here, $-q, \hbar, |v(E)|, \omega, \epsilon_{\text{free space}}, c$ 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:

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

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

Then, one has:

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

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

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

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

Further, one notes that, as $E \rightarrow \infty$, Forouhi and Bloomer (FB)^[4] claimed that $\kappa(E \rightarrow \infty) \rightarrow$ 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: $\sigma_0(E)$ and $\alpha(E)$, given in Eq. (16), both go to 0 as E^{-2} .

Now, an improved Forouhi-Bloomer parameterization model (FB-PM), used to determine the expressions of the optical coefficients in the degenerate $n^+(p^+) - p(n) X(x)$ - crystalline alloy, is now proposed as follows. Then, if denoting the functions $G(E)$ and $F(E)$ and by:

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

$$\begin{aligned} \kappa(E, N, r_{d(a)}, x, T) &= G(E) \times E_{gn1(gp1)}^{3/2} \times (E^* \equiv E - E_{gn1(gp1)})^{1/2}, \text{ for } E_{gn1(gp1)} \leq E \leq 2.3 \text{ eV,} \\ &= F(E) \times (E^* \equiv E - E_{gn1(gp1)})^2, \text{ for } E \geq 2.3 \text{ eV,} \end{aligned} \quad (20)$$

being equal to 0 for $E^* = 0$ (or for $E = E_{gn1(gp1)}$), and also going to 0 as E^{-1} as $E \rightarrow \infty$, 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 $E \rightarrow \infty$, since $n(E \rightarrow \infty, r_{d(a)}, x) \rightarrow n_\infty(r_{d(a)}, x) = \sqrt{\varepsilon(r_{d(a)}, x)} \times \frac{\omega_T}{\omega_L}$, $\omega_T = 5.1 \times 10^{13} \text{ s}^{-1}$ [5] and $\omega_L = 8.9755 \times 10^{13} \text{ s}^{-1}$.

Here, the other parameters are determined by:

$$\begin{aligned} X_i(E_{gn1(gp1)}) &= \frac{A_i}{Q_i} \times \left[-\frac{B_i^2}{2} + E_{gn1(gp1)} B_i - E_{gn1(gp1)}^2 + C_i \right], \\ Y_i(E_{gn1(gp1)}) &= \frac{A_i}{Q_i} \times \left[\frac{B_i \times (E_{gn1(gp1)}^2 + C_i)}{2} - 2E_{gn1(gp1)} C_i \right], \quad Q_i = \frac{\sqrt{4C_i - B_i^2}}{2}, \text{ where, for } i=(1, 2, 3, \\ &\text{and } 4), A_i = 1.154 \times A_{i(FB)} = 4.7314 \times 10^{-4}, 0.2314, 0.1118 \text{ and } 0.0116, \end{aligned}$$

$B_i \equiv B_{i(\text{FB})} = 5.871, 6.154, 9.679$ and 13.232 , and $C_i \equiv C_{i(\text{FB})} = 8.619, 9.784, 23.803$, 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 $\mathbf{X(x)} \equiv \text{GaSb}_{1-x}\text{Te}_x$ - 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:

$$T=0\text{K}, \quad N^* = 0 \quad \text{or} \quad N = N_{\text{CDn(CDp)}}, \quad \text{giving rise to:}$$

$$E_{\text{gn1(gp1)}}(N^* = 0, r_{\text{d(a)}}, x, T = 0) = E_{\text{gn1(gp1)}}(r_{\text{d(a)}}, x) = E_{\text{gno(gp0)}}(r_{\text{d(a)}}, x).$$

Then, in this MIT-case, if $E = E_{\text{gn1(gp1)}}(r_{\text{d(a)}}, x) = E_{\text{gno(gp0)}}(r_{\text{d(a)}}, x)$, which can be defined as the critical photon energy: $E \equiv E_{\text{CPE}}(r_{\text{d(a)}}, x)$, one obtains: $\kappa_{\text{MIT}}(r_{\text{d(a)}}, x) = 0$ from Eq. (20), and from Eq. (16): $\varepsilon_{2(\text{MIT})}(r_{\text{d(a)}}, x) = 0$, $\sigma_{\text{O}(\text{MIT})}(r_{\text{d(a)}}, x) = 0$ and $\alpha_{\text{MIT}}(r_{\text{d(a)}}, x) = 0$, and the other functions such as : $n_{\text{MIT}}(r_{\text{d(a)}}, x)$ from Eq. (21), and $\varepsilon_{1(\text{MIT})}(r_{\text{d(a)}}, x)$ and $R_{\text{MIT}}(r_{\text{d(a)}}, x)$ from Eq. (16) decrease with increasing $r_{\text{d(a)}}$ and E_{CPE} , as those investigated in Table 1 in Appendix 1.

B. Optical coefficients, obtained as $E \rightarrow \infty$

In Eq. (21), at any T , the choice of the real refraction index: $n(E \rightarrow \infty, r_{\text{d(a)}}, x, T) = n_{\infty}(r_{\text{d(a)}}, x) = \sqrt{\varepsilon(r_{\text{d(a)}}, x)} \times \frac{\omega_T}{\omega_L}$, $\omega_T = 5.1 \times 10^{13} \text{ s}^{-1}$ [5] and $\omega_L = 8.9755 \times 10^{13} \text{ s}^{-1}$, 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 ($E \rightarrow \infty$), we obtain: $\kappa_{\infty}(r_{\text{d(a)}}, x) \rightarrow 0$ and $\varepsilon_{2,\infty}(r_{\text{d(a)}}, x) \rightarrow 0$, as E^{-1} , so that $\varepsilon_{1,\infty}(r_{\text{d(a)}}, x)$, $\sigma_{\text{O},\infty}(r_{\text{d(a)}}, x)$, $\alpha_{\infty}(r_{\text{d(a)}}, x)$ and $R_{\infty}(r_{\text{d(a)}}, x)$ go to their appropriate limiting constants for $T=0\text{K}$, as those investigated in Table 2 in Appendix 1.

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

In the P(B)-X(x)-system, at $T=0\text{K}$ and $N = N_{\text{CDn(CDp)}}(r_{\text{P(B)}}, x)$, our numerical results of n , κ , ε_1 and ε_2 are obtained from Equations (21, 20, 16), respectively, and expressed as functions of $E [\geq E_{\text{CPE}}(r_{\text{P(B)}}, x)]$ 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 $E=3.2\text{ eV}$ and $T=20\text{ K}$, for given $r_{\text{d(a)}}$ and x , and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of $\eta_{\text{n(p)}} (>> 1, \text{degenerate case})$, $E_{\text{gn1(gp1)}}$, 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 $E=3.2\text{ eV}$ and $N = 10^{20}\text{ cm}^{-3}$, for given $r_{\text{d(a)}}$ and x , and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of $\eta_{\text{n(p)}} (>> 1, \text{degenerate case})$, $E_{\text{gn1(gp1)}}$, 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 $\mathbf{X(x)} \equiv \mathbf{GaSb_{1-x}Te_x}$ - crystalline alloy, by basing on our two recent works [1, 2], for a given x , and with an increasing $r_{\text{d(a)}}$, the optical coefficients have been determined, as functions of the photon energy E , total impurity density N , the donor (acceptor) radius $r_{\text{d(a)}}$, concentration x , and temperature T .

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

Further, we also showed that $N_{\text{CDn(NDp)}}$ is just the density of carriers localized in exponential band tails, with a precision of the order of 2.87×10^{-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: $N^*(N, r_{\text{d(a)}}, x) \equiv N - N_{\text{CDn(NDp)}}(r_{\text{d(a)}}, x)$, 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 impurity density in Metal-Insulator Transition, obtained in n(p)-type degenerate $\text{InSb}_{1-x}\text{P}_x(\text{As}_x)$, $\text{GaSb}_{1-x}\text{P}_x(\text{As}_x, \text{Te}_x)$, $\text{CdSe}_{1-x}\text{S}_x(\text{Te}_x)$ – 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 $\text{GaAs}_{1-x}\text{Te}_x$ - crystalline alloy, due to the new static dielectric constant-law and the generalized Mott criterium in the metal-insulator transition. (1). WJERT, 2024; 10(10): 122-147.
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 $E_{CPE} = E = E_{gno(gp0)}(r_{d(a)},x)$, 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: $\epsilon_{1(MIT)}(r_{d(a)},x)$ and $R_{MIT}(r_{d(a)},x)$, from Eq. (16), decrease (\searrow) with increasing (\nearrow) $r_{d(a)}$ and E_{CPE} .

Donor		P	Te	Sb	Sn
r_d (nm) [4]	\nearrow	0.110	0.132	0.136	0.140
At $x=0$,					
E_{CPE} in meV	\nearrow	809.22	809.98	810	810.02
n_{MIT}	\searrow	4.260	4.055	4.050	4.046
$\epsilon_{1(MIT)}$	\searrow	18.15	16.44	16.40	16.37
R_{MIT}	\searrow	0.384	0.365	0.365	0.364
At $x=0.5$,					
E_{CPE} in meV	\nearrow	1300.34	13.02.93	1303	1303.07
n_{MIT}	\searrow	3.818	3.622	3.618	3.614
$\epsilon_{1(MIT)}$	\searrow	14.57	13.12	13.09	13.06
R_{MIT}	\searrow	0.342	0.322	0.321	0.320
At $x=1$,					
E_{CPE} in meV	\nearrow	1790.37	1795.85	1796	1796.14
n_{MIT}	\searrow	3.367	3.182	3.178	3.174
$\epsilon_{1(MIT)}$	\searrow	11.34	10.12	10.10	10.07
R_{MIT}	\searrow	0.294	0.272	0.2713	0.2712
Acceptor		B	Ga	In	Cd
r_a (nm)	\nearrow	0.088	0.126	0.144	0.148

At $x=0$,

E_{CPE} in meV	↗	798.23	810	813.27	814.96
n_{MIT}	↘	4.874	4.050	3.949	3.904
$\epsilon_{1(MIT)}$	↘	23.75	16.40	15.60	15.24
R_{MIT}	↘	0.435	0.365	0.355	0.351

At $x=0.5$,

E_{CPE} in meV	↗	1285.74	1303	1308	1310
n_{MIT}	↘	4.400	3.618	3.521	3.479
$\epsilon_{1(MIT)}$	↘	19.36	13.09	12.40	12.10
R_{MIT}	↘	0.396	0.321	0.311	0.306

At $x=1$,

E_{CPE} in meV	↗	1770.5	1796	1803	1807
n_{MIT}	↘	3.917	3.178	3.086	3.045
$\epsilon_{1(MIT)}$	↘	15.34	10.10	9.52	9.27
R_{MIT}	↘	0.352	0.272	0.261	0.255

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

Donor		P	Te	Sb	Sn
At $x=0$,					
n_{∞}	↘	2.4604	2.2551	2.2507	2.2463
$\epsilon_{1,\infty}$	↘	6.0535	5.0853	5.0658	5.0459
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	11.2270	10.2900	10.2702	10.2500
α_{∞} in $(10^9 \times cm^{-1})$		= 2.1602			
R_{∞}	↘	0.1781	0.1487	0.1480	0.1474

At $x=0.5$,

n_{∞}	↘	2.324	2.130	2.126	2.121
$\varepsilon_{1,\infty}$	↘	5.399	4.536	4.518	4.501
$\sigma_{0,\infty}$	in $\frac{10^5}{\Omega \times cm}$ ↘	10.603	9.718	9.700	9.680
α_{∞}	in $(10^9 \times cm^{-1})=2.1602$				
R_{∞}	↘	0.159	0.130	0.1297	0.1291

At $x=1$,

n_{∞}	↘	2.178	1.997	1.9928	1.989
$\varepsilon_{1,\infty}$	↘	4.746	3.986	3.971	3.955
$\sigma_{0,\infty}$	in $\frac{10^5}{\Omega \times cm}$ ↘	9.940	9.111	9.093	9.075
α_{∞}	in $(10^9 \times cm^{-1})= 2.1602$				
R_{∞}	↘	0.137	0.1106	0.1100	0.109

Acceptor	B	Ga	In	Cd
----------	---	----	----	----

At $x=0$,

n_{∞}	↘	3.067	2.251	2.152	2.108
$\varepsilon_{1,\infty}$	↘	9.407	5.066	4.629	4.444
$\sigma_{0,\infty}$	in $\frac{10^5}{\Omega \times cm}$ ↘	13.99	10.27	9.818	9.619
α_{∞}	in $(10^9 \times cm^{-1}) = 2.1602$				
R_{∞}	↘	0.258	0.148	0.133	0.127

At $x=0.5$,

n_{∞}	↘	2.897	2.126	2.032	1.991
$\varepsilon_{1,\infty}$	↘	8.390	4.518	4.129	3.963
$\sigma_{0,\infty}$	in $\frac{10^5}{\Omega \times cm}$ ↘	13.22	9.700	9.272	9.084
α_{∞}	in $(10^9 \times cm^{-1})= 2.1602$				
R_{∞}	↘	0.237	0.130	0.116	0.110

At $x=1$,

n_{∞}	↘	2.715	1.993	1.905	1.866
$\varepsilon_{1,\infty}$	↘	7.374	3.971	3.629	3.483

$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$ ↘	12.39	9.093	8.693	8.517
α_∞ in $(10^9 \times cm^{-1})$	= 2.1602			
R_∞ ↘	0.213	0.110	0.097	0.091

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 $\epsilon_2 = 0$ at $E = E_{CPE}(r_p, x)$, and $\kappa \rightarrow 0$ and $\epsilon_2 \rightarrow 0$ as $E \rightarrow \infty$.

E in eV	n	κ	ϵ_1	ϵ_2
At x=0,				
$E_{CPE} = 0.80922$	4.2605	0	18.1518	0
2	5.537	0.136	30.642	1.505
2.5	6.652	1.082	43.074	14.398
3	5.978	3.942	20.196	47.138
3.5	4.100	3.770	2.599	30.917
4	4.327	3.082	9.229	26.671
4.5	4.855	4.433	3.928	43.046
5	2.255	5.871	-29.379	26.482
5.5	0.636	3.980	-15.434	5.061
6	0.920	2.872	-7.404	5.285
...				
10^{22}	2.4604	0	6.0535	0
At x=0.5,				
$E_{CPE} = 1.3003$	3.8178	0	14.5754	0
2	4.438	0.212	19.654	1.883
2.5	5.239	0.545	27.147	5.709
3	5.089	2.373	20.268	24.153
3.5	3.961	2.519	9.341	19.959
4	4.124	2.206	12.145	18.198
4.5	4.530	3.331	9.425	30.186

5	2.525	4.575	-14.557	23.108
5.5	1.186	3.190	-8.769	7.569
6	1.356	2.354	-3.703	6.388
...				
10²²	2.3237	0	5.3996	0

At x=1,

E_{CPE} =1.7904	3.3672	0	11.3378	0
2	3.514	0.188	12.315	1.319
2.5	4.045	0.191	16.325	1.542
3	4.228	1.202	16.435	10.164
3.5	3.691	1.522	11.307	11.235
4	3.823	1.478	12.428	11.299
4.5	4.137	2.389	11.405	19.767
5	2.659	3.444	-4.786	18.315
5.5	1.584	2.489	-3.687	7.884
6	1.666	1.889	-0.793	6.294
...				
10²²	2.1784	0	4.7456	0

E in eV	<i>n</i>	<i>κ</i>	ϵ_1	ϵ_2
---------	----------	----------	--------------	--------------

Table 3p: In the B-X(x)-system, and at T=0K and $N = N_{CDP}(r_B, x)$, 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 $E [\geq E_{CPE}(r_B, x)]$ and x, noting that (i) $\kappa = 0$ and $\epsilon_2 = 0$ at $E = E_{CPE}(r_B, x)$, and $\kappa \rightarrow 0$ and $\epsilon_2 \rightarrow 0$ as $E \rightarrow \infty$.

E in eV	<i>n</i>	<i>κ</i>	ϵ_1	ϵ_2
At x=0,				
E_{CPE} =0.7982	4.8740	0	23.7557	0
2	6.167	0.134	38.019	1.650
2.5	7.289	1.096	51.934	15.984
3	6.602	3.982	27.731	52.581

3.5	4.706	3.801	7.696	35.771
4	4.934	3.103	14.720	30.623
4.5	5.466	4.459	9.991	48.745
5	2.851	5.901	-26.697	33.657
5.5	1.225	3.998	-14.485	9.800
6	1.512	2.884	-6.032	8.725
...				
10²²	3.0670	0	9.4067	0

At $x=0.5$,

$E_{CPE} = 1.2857$	4.3998	0	19.3582	0
2	5.037	0.211	25.329	2.123
2.5	5.846	0.558	33.868	6.527
3	5.684	2.414	26.480	27.441
3.5	4.536	2.553	14.055	23.159
4	4.701	2.230	17.124	20.965
4.5	5.109	3.362	14.807	34.357
5	3.088	4.611	-11.731	28.481
5.5	1.741	3.212	-7.287	11.185
6	1.914	2.369	-1.949	9.070
...				
10²²	2.8966	0	8.3905	0

At $x=1$,

$E_{CPE} = 1.7705$	3.9167	0	15.3404	0
2	4.079	0.193	16.605	1.575
2.5	4.620	0.201	21.306	1.862
3	4.794	1.242	21.439	11.906
3.5	4.235	1.557	15.513	13.194
4	4.368	1.505	16.814	13.144
4.5	4.685	2.424	16.073	22.717
5	3.187	3.486	-1.995	22.226
5.5	2.102	2.516	-1.912	10.575

6	2.187	1.907	1.146	8.341
...				
10²²	2.7156	0	7.3743	0

E in eV	<i>n</i>	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 $\eta_n (>> 1, \text{degenerate case})$, E_{gn1} , *n*, κ , ϵ_1 and ϵ_2 , obtained as functions of N, being represented by the arrows: ↗ and ↘, noting that both η_n and E_{gn1} increase with increasing N.

N (10^{18} cm^{-3}) ↗	15	26	60	100
-----------------------------------	----	----	----	-----

x=0

For $r_d = r_{sb}$,

$\eta_n \gg 1$	↗	316	457	798	1121
E_{gn1} in eV	↗	0.688	0.733	0.900	1.102
<i>n</i>	↘	5.115	5.080	4.945	4.773
κ	↘	4.676	4.512	3.923	3.262
ϵ_1	↗	4.300	5.450	9.063	12.146
ϵ_2	↘	47.837	45.837	38.793	31.143

For $r_d = r_{sn}$,

$\eta_n \gg 1$	↗	316	457	798	1121
E_{gn1} in eV	↗	0.691	0.736	0.904	1.108
<i>n</i>	↘	5.109	5.073	4.937	4.764
κ	↘	4.668	4.501	3.908	3.244
ϵ_1	↗	4.312	5.477	9.100	12.172
ϵ_2	↘	47.698	45.671	38.583	30.915

x=0.5

For $r_d = r_{Sb}$,

$\eta_n \gg 1$	↗	137	198	345	486
E_{gn1} in eV	↗	1.281	1.313	1.414	1.526
n	↘	4.491	4.462	4.371	4.266
κ	↘	2.729	2.639	2.365	2.077
ε_1	↗	12.721	12.949	13.510	13.887
ε_2	↘	24.515	23.551	20.675	17.718

For $r_d = r_{Sn}$,

$\eta_n \gg 1$	↗	137	198	345	486
E_{gn1} in eV	↗	1.282	1.314	1.415	1.528
n	↘	4.486	4.457	4.365	4.260
κ	↘	2.727	2.636	2.361	2.072
ε_1	↗	12.690	12.918	13.480	13.856
ε_2	↘	24.468	23.499	20.613	17.651

x=1

For $r_d = r_{Sb}$,

$\eta_n \gg 1$	↗	91	133	235	331
E_{gn1} in eV	↗	1.792	1.819	1.900	1.988
n	↘	3.877	3.850	3.769	3.680
κ	↘	1.469	1.413	1.252	1.089
ε_1	↘	12.870	12.823	12.635	12.353
ε_2	↘	11.392	10.878	9.438	8.017

For $r_d = r_{Sn}$,

$\eta_n \gg 1$	↗	91	133	235	331
E_{gn1} in eV	↗	1.793	1.820	1.901	1.989
n	↘	3.872	3.845	3.764	3.674
κ	↘	1.468	1.411	1.250	1.087

ε_1	\searrow	12.839	12.792	12.602	12.320
ε_2	\searrow	11.371	10.855	9.412	7.989
<hr/>					
$N (10^{18} \text{ cm}^{-3})$	\nearrow	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: \nearrow and \searrow , noting that both η_p and E_{gp1} increase with increasing N.

$N (10^{18} \text{ cm}^{-3})$	\nearrow	15	26	60	100
-------------------------------	------------	----	----	----	-----

x=0

For $r_a = r_{In}$,

$\eta_p \gg 1$	\nearrow	303	445	789	1114
E_{gp1} in eV	\nearrow	0.769	0.850	1.001	1.378
<hr/>					
n	\searrow	4.952	4.886	4.676	4.430
κ	\searrow	4.381	4.093	3.267	2.461
ε_1	\nearrow	5.331	7.122	11.191	13.563
ε_2	\searrow	43.387	40.000	30.548	21.808

For $r_a = r_{Cd}$,

$\eta_p \gg 1$	\nearrow	301	444	788	1113
E_{gp1} in eV	\nearrow	0.784	0.870	1.132	1.418
<hr/>					
n	\searrow	4.896	4.826	4.605	4.349
κ	\searrow	4.326	4.023	3.170	2.553
ε_1	\nearrow	5.254	7.106	11.156	13.376
ε_2	\searrow	42.367	38.832	29.199	20.467

x=0.5

For $r_a = r_{In}$,

$\eta_p \gg 1$	↗	123.8	187	337	479
E_{gp1} in eV	↗	1.196	1.206	1.265	1.345
n	↘	4.474	4.465	4.412	4.340
κ	↘	2.978	2.949	2.777	2.552
ε_1	↗	11.142	11.240	11.759	12.327
ε_2	↘	26.648	26.330	24.505	22.152

For $r_a = r_{Cd}$,

$\eta_p \gg 1$	↗	122	185	336	478
E_{gp1} in eV	↗	1.205	1.218	1.283	1.368
n	↘	4.424	4.413	4.355	4.278
κ	↘	2.950	2.912	2.725	2.488
ε_1	↗	10.870	10.990	11.541	12.111
ε_2	↘	26.098	25.703	23.731	21.285

x=1

For $r_a = r_{In}$,

$\eta_p \gg 1$	↗	73	118	223	321
E_{gp1} in eV	↗	1.755	1.773	1.837	1.912
n	↘	3.825	3.808	3.744	3.369
κ	↘	1.547	1.510	1.377	1.229
ε_1	↘	12.239	12.221	12.124	11.949
ε_2	↘	11.840	11.503	10.311	9.017

For $r_a = r_{Cd}$,

$\eta_p \gg 1$	↗	70	116	222	320
E_{gp1} in eV	↗	1.761	1.780	1.848	1.926
n	↘	3.781	3.762	3.695	3.616
κ	↘	1.534	1.494	1.355	1.203
ε_1	↘	11.940	11.920	11.815	11.629
ε_2	↘	11.602	11.245	10.014	8.700

$N (10^{18} \text{ cm}^{-3})$	\nearrow	15	26	60	100
-------------------------------	------------	----	----	----	-----

Table 5n: In the X(x)-system, at $E=3.2 \text{ eV}$ and $N = 10^{20} \text{ cm}^{-3}$, 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: \nearrow and \searrow , noting that both η_n and E_{gn1} decrease with increasing T .

T in K	\nearrow	20	50	100	300
--------	------------	----	----	-----	-----

x=0

For $r_d = r_{Sb}$,

$\eta_n \gg 1$	\searrow	1121	448	224	75
E_{gn1} in eV	\searrow	1.102	1.098	1.085	1.006
n	\nearrow	4.773	4.777	4.788	4.855
κ	\nearrow	3.262	3.276	3.315	3.567
ε_1	\searrow	12.146	12.093	11.939	10.823
ε_2	\nearrow	31.143	31.297	31.716	34.638

For $r_d = r_{Sn}$,

$\eta_n \gg 1$	\searrow	1121	448	224	75
E_{gn1} in eV	\searrow	1.108	1.104	1.091	1.012
n	\nearrow	4.764	4.768	4.779	4.846
κ	\nearrow	3.244	3.258	3.297	3.548
ε_1	\searrow	12.172	12.119	11.967	10.894
ε_2	\nearrow	30.915	31.069	31.511	34.394

x=0.5

For $r_d = r_{Sb}$,

$\eta_n \gg 1$	\searrow	486	194	97	32
E_{gn1} in eV	\searrow	1.526	1.519	1.500	1.397

n	\nearrow	4.266	4.273	4.290	4.386
κ	\nearrow	2.077	2.094	2.141	2.410
ε_1	\searrow	13.887	13.870	13.822	13.430
ε_2	\nearrow	17.718	17.899	18.372	21.145

For $r_d = r_{Sn}$,

$\eta_n \gg 1$	\searrow	485.9	194	97	32
E_{gn1} in eV	\searrow	1.528	1.521	1.502	1.399

n	\nearrow	4.260	4.267	4.284	4.380
κ	\nearrow	2.072	2.089	2.136	2.405
ε_1	\searrow	13.856	13.839	13.792	13.403
ε_2	\nearrow	17.651	17.831	18.303	21.069

$x=1$

For $r_d = r_{Sb}$,

$\eta_n \gg 1$	\searrow	331	132	66	22
E_{gn1} in eV	\searrow	1.988	1.978	1.953	1.825

n	\nearrow	3.680	3.690	3.715	3.844
κ	\nearrow	1.089	1.107	1.153	1.402
ε_1	\nearrow	12.353	12.389	12.474	12.813
ε_2	\nearrow	8.017	8.172	8.564	10.779

For $r_d = r_{Sn}$,

$\eta_n \gg 1$	\searrow	331	132	66	22
E_{gn1} in eV	\searrow	1.989	1.979	1.954	1.826

n	\nearrow	3.674	3.685	3.710	3.839
κ	\nearrow	1.087	1.105	1.150	1.399
ε_1	\nearrow	12.320	12.356	12.441	12.781
ε_2	\nearrow	7.989	8.145	8.536	10.746

T in K	\nearrow	20	50	100	300
--------	------------	----	----	-----	-----

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

T in K		20	50	100	300
x=0					

For $r_a = r_{In}$,					
$\eta_p \gg 1$	↘	1114	446	223	74
E_{gp1} in eV	↘	1.378	1.373	1.361	1.282
n	↗	4.430	4.434	4.445	4.516
κ	↗	2.461	2.473	2.507	2.727
ϵ_1	↘	13.563	13.540	13.472	12.960
ϵ_2	↗	21.808	21.932	22.290	24.635

For $r_a = r_{Cd}$,					
$\eta_p \gg 1$	↘	1113	445	223	74
E_{gp1} in eV	↘	1.418	1.414	1.401	1.322
n	↗	4.349	4.353	4.364	4.436
κ	↗	2.353	2.365	2.400	2.613
ϵ_1	↘	13.375	13.356	13.298	12.853
ϵ_2	↗	20.467	20.586	20.930	23.185

x=0.5					

For $r_a = r_{In}$,					
$\eta_p \gg 1$	↘	479	192	96	32
E_{gp1} in eV	↘	1.345	1.337	1.319	1.215
n	↗	4.340	4.347	4.364	4.456
κ	↗	2.552	2.572	2.623	2.920
ϵ_1	↘	12.327	12.282	12.160	11.330

ε_2	\nearrow	22.152	22.358	22.895	26.029
-----------------	------------	--------	--------	--------	--------

 For $r_a = r_{Cd}$,

$\eta_p \gg 1$	\searrow	478	191	96	32
E_{gp1} in eV	\searrow	1.368	1.361	1.342	1.239

n	\nearrow	4.278	4.284	4.301	4.394
κ	\nearrow	2.488	2.507	2.558	2.852
ε_1	\searrow	12.111	12.069	11.956	11.177
ε_2	\nearrow	21.285	21.485	22.008	25.064

x=1

 For $r_a = r_{In}$,

$\eta_p \gg 1$	\searrow	321	128	64	21
E_{gp1} in eV	\searrow	1.912	1.902	1.878	1.749

n	\nearrow	3.669	3.679	3.704	3.831
κ	\nearrow	1.229	1.248	1.296	1.560
ε_1	\nearrow	11.949	11.975	12.037	12.244
ε_2	\nearrow	9.017	9.183	9.601	11.952

 For $r_a = r_{Cd}$,

$\eta_p \gg 1$	\searrow	320	128	64	21
E_{gp1} in eV	\searrow	1.926	1.916	1.891	1.763

n	\nearrow	3.616	3.626	3.651	3.779
κ	\nearrow	1.203	1.222	1.269	1.531
ε_1	\nearrow	11.629	11.657	11.720	11.938
ε_2	\nearrow	8.700	8.862	9.270	11.569

T in K	\nearrow	20	50	100	300
--------	------------	----	----	-----	-----
