



**OPTICAL COEFFICIENTS IN THE N(P)-TYPE DEGENERATE
GaSb(1-x) P(x)-CRYSTALLINE ALLOY, DUE TO THE NEW STATIC
DIELECTRIC CONSTANT-LAW AND THE GENERALIZED MOTT
CRITERIUM IN THE METAL-INSULATOR TRANSITION. (11)**

Huynh Van Cong*, Paul Blaise and Michel Cayrol

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 23/09/2024

Article Revised on 14/10/2024

Article Accepted on 02/11/2024



***Corresponding Author**

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

9a). Furthermore, we also showed that $N_{CDn(NDp)}$ is just the density of carriers localized in exponential band tails, with a precision of the order of 2.92×10^{-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.

KEYWORDS: GaSb_{1-x}P_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 $X(x) \equiv \text{GaSb}_{1-x}\text{P}_x$ - 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:

$$m_{c(v)}(x)/m_o = 0.13 (0.5) \times x + 0.047 (0.3) \times (1 - x) \quad (1)$$

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

$$\epsilon_o(x) = 11.1 \times x + 15.69 \times (1 - x). \quad (2)$$

(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:

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

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

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

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

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

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

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

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

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

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

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

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:

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

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

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

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

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

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 2.92×10^{-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:

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

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

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

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

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

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:

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

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

$$\Delta E_{\text{gn}}(N, r_d, x) = \Delta E_{\text{gno}}(N, r_d, x) \times \{1.5 \times x + 0.5 \times (1 - x)\}, \tag{14n}$$

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:

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

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

$$\Delta E_{\text{gp}}(N, r_a, x) = \Delta E_{\text{gpo}}(N, r_a, x) \times \{10 \times x + 8 \times (1 - x)\}, \tag{14p}$$

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:

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

where $E_{\text{gin(gp1)}} \cdot [+E_{\text{Fn}}, -E_{\text{Fp}}] \geq 0$, 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: $E_{\text{gn1(gp1)}}(r_{d(a)}, x) = E_{\text{gno(gp0)}}(r_{d(a)}, x)$, according to: $N = N_{\text{CDn(NDp)}}(r_{d(a)}, x)$.

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_0 , by^[2]

$$\alpha(E, N, r_{d(a)}, x, T) \equiv \frac{\hbar q^2 \times |v(E)|^2}{n(E) \times \varepsilon_{\text{free space}} \times c E} \times J(E^*) = \frac{E \times \varepsilon_2(E)}{\hbar c n(E)} \equiv \frac{2E \times \kappa(E)}{\hbar c} \equiv \frac{4\pi \sigma_0(E)}{c n(E) \times \varepsilon_{\text{free space}}},$$

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

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

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

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

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

Then, one has:

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

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

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

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

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

Here, the other parameters are determined by:

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

$$Y_i(E_{gn1(gp1)}) = \frac{A_i}{Q_i} \times \left[\frac{B_i \times (E_{gn1(gp1)}^2 + C_i)}{2} - 2E_{gn1(gp1)} C_i \right], \quad Q_i = \frac{\sqrt{4C_i - B_i^2}}{2}, \text{ where, for } i=(1, 2, 3,$$

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 $\mathbf{X(x)} \equiv \mathbf{GaSb_{1-x}P_x}$ - 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:

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

Then, in this MIT-case, if $E = E_{gn1(gp1)}(r_{d(a)}, x) = E_{gno(gp0)}(r_{d(a)}, x)$, 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 $E \rightarrow \infty$

In Eq. (21), at any T , the choice of the real refraction index: $n(E \rightarrow \infty, r_{d(a)}, x, T) = n_{\infty}(r_{d(a)}, x) = \sqrt{\varepsilon(r_{d(a)}, x)} \times \frac{\omega_T}{\omega_L}$, $\omega_T = 5.1 \times 10^{13} \text{ s}^{-1}$ [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: $\kappa_{\infty}(r_{d(a)}, x) \rightarrow 0$ and $\varepsilon_{2,\infty}(r_{d(a)}, x) \rightarrow 0$, 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(B)-X(x)-system, as functions of E

In the P(B)-X(x)-system, at $T=0K$ and $N = N_{CDn(CDp)}(r_{P(B)}, x)$, our numerical results of n , κ , ε_1 and ε_2 are obtained from Equations (21, 20, 16), respectively, and expressed as functions of $E [\geq E_{CPE}(r_{P(B)}, x)]$ 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 $E=3.2$ 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 $\eta_{n(p)} (>> 1, \text{degenerate case})$, $E_{gn1(gp1)}$, 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.

Variations of various optical coefficients as functions of T

In the X(x)-system, at $E=3.2$ eV and $N = 10^{20} \text{cm}^{-3}$, for given $r_{d(a)}$ and x , and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of $\eta_{n(p)} (>> 1, \text{degenerate case})$, $E_{gn1(gp1)}$, 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 $\mathbf{X(x)} \equiv \mathbf{GaSb_{1-x}P_x}$ - 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 2.92×10^{-7} , as that given in Table 4 of Ref.^[1], according to a definition of the effective density of electrons (holes) given in parabolic conduction (valence) bands by: $N^*(N, r_{d(a)}, x) \equiv N - N_{CDn(NDp)}(r_{d(a)}, x)$, as defined in Eq. (9d).

In summary, due to the new $\varepsilon(r_{d(a)}, x)$ -law and to the effective density of electrons (holes) given in parabolic conduction (valence) bands $N^*(N, r_{d(a)}, x)$, for a given x , and with an increasing $r_{d(a)}$, the numerical results of all the optical coefficients, obtained in appropriated physical conditions (E, N, T), and calculated by using Equations (15, 16, 20, 21), are reported in Tables 1, 2, 3n, 3p, 4n, 4p, 5n, and 5p in Appendix 1.

REFERENCES

1. Van Cong, H. Critical 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. & Debais, 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	1300.99	1302.95	1303	1303.05
n_{MIT}	\searrow	3.767	3.576	3.572	3.568
$\epsilon_{1(MIT)}$	\searrow	14.19	12.79	12.76	12.73
R_{MIT}	\searrow	0.337	0.317	0.31647	0.31602

At $x=1$,					
E_{CPE} in meV	\nearrow	1791.70	1795.89	1796	1796.11
n_{MIT}	\searrow	3.257	3.082	3.078	3.074
$\epsilon_{1(MIT)}$	\searrow	10.61	9.50	9.47	9.45
R_{MIT}	\searrow	0.281	0.260	0.2597	0.2592

Acceptor		B	Ga	In	Cd
r_a (nm)	\nearrow	0.088	0.126	0.144	0.148

At $x=0$,					
E_{CPE} in meV	\nearrow	798.23	810	813.27	814.96
n_{MIT}	\searrow	4.874	4.050	3.949	3.904
$\epsilon_{1(MIT)}$	\searrow	23.75	16.40	15.60	15.24
R_{MIT}	\searrow	0.435	0.365	0.355	0.351

At $x=0.5$,

E_{CPE} in meV	↗	1281.47	1303	1309	1312
n_{MIT}	↘	4.340	3.572	3.477	3.434
$\epsilon_{1(MIT)}$	↘	18.83		12.76	12.09
R_{MIT}	↘	0.391	0.316	0.306	0.301

At $x=1$,

E_{CPE} in meV	↗	1756.81	1796	1807	1812
n_{MIT}	↘	3.789	3.078	2.988	2.948
$\epsilon_{1(MIT)}$	↘	14.36	9.47	8.93	8.69
R_{MIT}	↘	0.339	0.260	0.248	0.243

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_{∞}	↘	2.2733	2.0836	2.0796	2.0755
$\epsilon_{1,\infty}$	↘	5.1681	4.3415	4.3248	4.3078
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	10.3734	9.5077	9.4894	9.4708
α_{∞} in $(10^9 \times cm^{-1})$		= 2.1602			
R_{∞}	↘	0.1513	0.1235	0.1229	0.1223

At $x=1$,

n_{∞}	↘	2.0694	1.8967	1.8931	1.8894
$\varepsilon_{1,\infty}$	↘	4.2826	3.5976	3.5838	3.5697
$\sigma_{0,\infty}$	in $\frac{10^5}{\Omega \times cm}$ ↘	9.4430	8.6550	8.6383	8.6214
α_{∞}	in $(10^9 \times cm^{-1})= 2.1602$				
R_{∞}	↘	0.1214	0.0958	0.0953	0.0947

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_{∞}	↘	2.834	2.080	1.988	1.948
$\varepsilon_{1,\infty}$	↘	8.031	4.325	3.952	3.794
$\sigma_{0,\infty}$	in $\frac{10^5}{\Omega \times cm}$ ↘	12.93	9.489	9.071	8.888
α_{∞}	in $(10^9 \times cm^{-1})= 2.1602$				
R_{∞}	↘	0.229	0.123	0.109	0.103

At $x=1$,

n_{∞}	↘	2.580	1.893	1.810	1.773
$\varepsilon_{1,\infty}$	↘	6.655	3.584	3.275	3.144
$\sigma_{0,\infty}$	in $\frac{10^5}{\Omega \times cm}$ ↘	11.77	8.638	8.258	8.090
α_{∞}	in $(10^9 \times cm^{-1})= 2.1602$				
R_{∞}	↘	0.195	0.095	0.083	0.078

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 $\kappa \rightarrow 0$ and $\varepsilon_2 \rightarrow 0$ 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,				
$E_{CPE} = 1.3010$	3.7670	0	14.1903	0
2	4.387	0.212	19.199	1.862
2.5	5.187	0.544	26.607	5.646
3	5.038	2.371	19.757	23.891
3.5	3.910	2.518	8.951	19.693
4	4.074	2.205	11.736	17.967
4.5	4.480	3.330	8.978	29.836
5	2.475	4.574	-14.792	22.643
5.5	1.137	3.189	-8.877	7.251
6	1.307	2.354	-3.832	6.152
...				
10^{22}	2.2733	0	5.1681	0

At $x=1$,

$E_{CPE}=1.7917$	3.2573	0	10.6103	0
2	3.403	0.187	11.549	1.274
2.5	3.933	0.190	15.436	1.494
3	4.117	1.199	15.516	9.876
3.5	3.581	1.519	10.518	10.885
4	3.713	1.476	11.608	10.962
4.5	4.027	2.387	10.520	19.224
5	2.551	3.441	-5.332	17.554
5.5	1.476	2.487	-4.007	7.343
6	1.558	1.888	-1.136	5.883
...				
10^{22}	2.0694	0	4.2826	0

E in eV	n	κ	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 $\varepsilon_2 = 0$ at $E = E_{CPE}(r_B, x)$, and $\kappa \rightarrow 0$ and $\varepsilon_2 \rightarrow 0$ as $E \rightarrow \infty$.

E in eV	n	κ	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} = 1.2815	4.3397	0	18.8329	0
2	4.982	0.210	24.777	2.096
2.5	5.794	0.562	33.251	6.514
3	5.627	2.426	25.784	27.304
3.5	4.473	2.563	13.443	22.930
4	4.640	2.237	16.516	20.755
4.5	5.049	3.371	14.128	34.038
5	3.022	4.622	-12.231	27.938
5.5	1.673	3.219	-7.562	10.769
6	1.847	2.373	-2.222	8.767
...				
10²²	2.8339	0	8.0308	0

At x=1,

E_{CPE} = 1.7568	3.7893	0	14.3590	0
2	3.963	0.196	15.668	1.557
2.5	4.511	0.209	20.304	1.886
3	4.677	1.269	20.268	11.876
3.5	4.105	1.582	14.344	12.989
4	4.237	1.523	15.636	12.908
4.5	4.557	2.449	14.769	22.317
5	3.045	3.516	-3.087	21.416
5.5	1.952	2.534	-2.610	9.896
6	2.040	1.919	0.477	7.830
...				
10²²	2.5797	0	6.6548	0

E in eV

n

κ

ε₁

ε₂

Table 4n: In the X(x)-system, at E=3.2 eV and T=20 K, for given r_d and x, and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of $\eta_n (\gg 1, \text{degenerate case})$, E_{gn1} , n, κ , ε_1 and ε_2 , obtained as functions of N, being represented by the arrows: ↗ and ↘, noting that both η_n and E_{gn1} increase with increasing N.

N (10^{18} cm^{-3})	↗	15	26	60	100
x=0					

For $r_d = r_{Sb}$,					
$\eta_n \gg 1$	↗	239	345	602	847
E_{gn1} in eV	↗	0.750	0.792	0.937	1.102
n	↘	5.066	5.032	4.914	4.771
κ	↘	4.450	4.297	3.797	3.253
ε_1	↗	5.865	6.857	9.727	12.181
ε_2	↘	45.093	43.253	37.322	31.041

For $r_d = r_{Sn}$,					
$\eta_n \gg 1$	↗	239	345	602	847
E_{gn1} in eV	↗	0.751	0.794	0.9398	1.109
n	↘	5.061	5.026	4.907	4.763
κ	↘	4.444	4.290	3.787	3.240
ε_1	↗	5.858	6.859	9.738	12.187
ε_2	↘	44.985	43.127	37.165	30.869

x=0.5					

For $r_d = r_{Sb}$,					
$\eta_n \gg 1$	↗	131	188	329	463
E_{gn1} in eV	↗	1.219	1.230	1.284	1.356
n	↘	4.500	4.490	4.442	4.378
κ	↘	2.907	2.875	2.720	2.521
ε_1	↗	11.796	11.895	12.333	12.808
ε_2	↘	26.167	25.822	24.169	22.072

For $r_d = r_{Sn}$,

$\eta_n \gg 1$	↗	130.6	188.6	329.5	463
E_{gn1} in eV	↗	1.220	1.232	1.286	1.358
n	↘	4.495	4.485	4.436	4.371
κ	↘	2.905	2.871	2.715	2.514
ε_1	↗	11.768	11.869	12.311	12.787
ε_2	↘	26.113	25.758	24.089	21.981

x=1

For $r_d = r_{Sb}$,

$\eta_n \gg 1$	↗	93	135	236	331
E_{gn1} in eV	↗	1.745	1.758	1.808	1.868
n	↘	3.823	3.810	3.762	3.701
κ	↘	1.568	1.541	1.437	1.314
ε_1	↘	12.155	12.145	12.085	11.970
ε_2	↘	11.991	11.745	10.813	9.728

For $r_d = r_{Sn}$,

$\eta_n \gg 1$	↗	93	134.6	235.7	331
E_{gn1} in eV	↗	1.746	1.759	1.809	1.870
n	↘	3.818	3.806	3.757	3.695
κ	↘	1.567	1.539	1.434	1.311
ε_1	↘	12.126	12.116	12.055	11.938
ε_2	↘	11.967	11.717	10.778	9.690

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

Table 4p: In the X(x)-system, at E=3.2 eV and T=20 K, for given r_d and x , and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of $\eta_p (\gg 1, \text{degenerate case})$, E_{gp1} , n , κ , ε_1 and ε_2 , obtained as functions of N, being represented by the arrows: ↗ and ↘, noting that both η_p and E_{gp1} increase with increasing N.

N (10^{18} cm^{-3})	↗	15	26	60	100
x=0					

For $r_a = r_{Ga}$,					
$\eta_p \gg 1$	↗	231	338	598	843
E_{gp1} in eV	↗	0.804	0.871	1.073	1.292
n	↘	5.023	4.968	4.798	4.606
κ	↘	4.257	4.020	3.353	2.697
ε_1	↗	7.111	8.523	11.784	13.941
ε_2	↘	42.766	39.941	32.179	24.846

For $r_a = r_{In}$,					
$\eta_p \gg 1$	↗	229	336	596	841
E_{gp1} in eV	↗	0.828	0.904	1.123	1.357
n	↘	4.904	4.842	4.656	4.448
κ	↘	4.170	3.908	3.198	2.518
ε_1	↗	6.661	8.172	11.458	13.451
ε_2	↘	40.902	37.848	29.780	22.400

For $r_a = r_{Cd}$,					
$\eta_p \gg 1$	↗	227	335	595	841
E_{gp1} in eV	↗	0.838	0.918	1.144	1.384
n	↘	4.852	4.787	4.594	4.380
κ	↘	4.134	3.861	3.133	2.443
ε_1	↗	6.455	8.000	11.294	13.214
ε_2	↘	40.116	36.971	28.788	21.402

x=0.5

For $r_a = r_{Ga}$,

$\eta_p \gg 1$	↗	114	175	319	455
E_{gp1} in eV	↗	1.258	1.287	1.383	1.492
n	↘	4.465	4.440	4.353	4.252
κ	↘	2.795	2.712	2.447	2.163
ε_1	↗	12.130	12.354	12.958	13.404
ε_2	↘	24.961	24.084	21.306	18.395

For $r_a = r_{In}$,

$\eta_p \gg 1$	↗	108	170	316	452
E_{gp1} in eV	↗	1.273	1.307	1.413	1.530
n	↘	4.360	4.331	4.234	4.125
κ	↘	2.752	2.657	2.368	2.067
ε_1	↗	11.442	11.693	12.320	12.741
ε_2	↘	23.998	23.015	20.055	17.055

For $r_a = r_{Cd}$,

$\eta_p \gg 1$	↗	105	168	314	450
E_{gp1} in eV	↗	1.280	1.315	1.425	1.546
n	↘	4.315	4.283	4.182	4.069
κ	↘	2.734	2.634	2.335	2.027
ε_1	↗	11.142	11.404	12.039	12.449
ε_2	↘	23.590	22.564	19.532	16.499

x=1

For $r_a = r_{Ga}$,

$\eta_p \gg 1$	↗	47	99	210	310
E_{gp1} in eV	↗	1.760	1.784	1.866	1.956
n	↘	3.808	3.785	3.703	3.613
κ	↘	1.536	1.486	1.319	1.148

ε_1	\searrow	12.143	12.117	11.975	11.735
ε_2	\searrow	11.700	11.246	9.771	8.293

For $r_a = r_{In}$,

$\eta_p \gg 1$	\nearrow	28	87	202	303
E_{gp1} in eV	\nearrow	1.771	1.795	1.883	1.979

n	\searrow	3.714	3.691	3.602	3.505
κ	\searrow	1.513	1.463	1.285	1.105
ε_1	\searrow	11.506	11.481	11.327	11.068
ε_2	\searrow	11.242	10.803	9.256	7.748

For $r_a = r_{Cd}$,

$\eta_p \gg 1$	\nearrow	13	80	197	299.7
E_{gp1} in eV	\nearrow	1.780	1.799	1.891	1.990

n	\searrow	3.669	3.650	3.559	3.459
κ	\searrow	1.495	1.455	1.271	1.087
ε_1	\searrow	11.227	11.207	11.049	10.781
ε_2	\searrow	10.968	10.604	9.045	7.523

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

Table 5n: In the X(x)-system, at E=3.2 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 $\eta_n (> 1, \text{degenerate case})$, 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	847	339	169	56
E_{gn1} in eV	\searrow	1.105	1.101	1.088	1.009

n	\nearrow	4.771	4.775	4.785	4.853
---	------------	-------	-------	-------	-------

κ	\nearrow	3.253	3.267	3.306	3.558
ε_1	\searrow	12.181	12.128	11.975	10.894
ε_2	\nearrow	31.041	31.195	31.639	34.533

For $r_d = r_{Sn}$,

$\eta_n \gg 1$	\searrow	847	339	169	56
E_{gn1} in eV	\searrow	1.109	1.105	1.092	1.013

n	\nearrow	4.763	4.767	4.778	4.845
κ	\nearrow	3.240	3.254	3.293	3.545
ε_1	\searrow	12.187	12.135	11.983	10.912
ε_2	\nearrow	30.869	31.023	31.465	34.349

x=0.5

For $r_d = r_{Sb}$,

$\eta_n \gg 1$	\searrow	463	185	92.6	31
E_{gn1} in eV	\searrow	1.356	1.349	1.330	1.226

n	\nearrow	4.378	4.384	4.401	4.494
κ	\nearrow	2.521	2.541	2.592	2.887
ε_1	\searrow	12.808	12.766	12.651	11.858
ε_2	\nearrow	22.072	22.278	22.815	25.952

For $r_d = r_{Sn}$,

$\eta_n \gg 1$	\searrow	463	185	92.6	31
E_{gn1} in eV	\searrow	1.358	1.351	1.333	1.229

n	\nearrow	4.371	4.378	4.395	4.488
κ	\nearrow	2.514	2.534	2.585	2.880
ε_1	\searrow	12.787	12.745	12.631	11.843
ε_2	\nearrow	21.981	22.186	22.722	25.851

x=1

For $r_d = r_{Sb}$,

$\eta_n \gg 1$	\searrow	331	133	66	22
E_{gn1} in eV	\searrow	1.868	1.858	1.834	1.705
n	\nearrow	3.701	3.711	3.736	3.862
κ	\nearrow	1.314	1.334	1.384	1.656
ε_1	\nearrow	11.970	11.991	12.040	12.174
ε_2	\nearrow	9.728	9.901	10.338	12.789

For $r_d = r_{Sn}$,					
$\eta_n \gg 1$	\searrow	331	132.6	66	22
E_{gn1} in eV	\searrow	1.870	1.860	1.835	1.707
n	\nearrow	3.695	3.706	3.730	3.857
κ	\nearrow	1.311	1.331	1.380	1.652
ε_1	\nearrow	11.938	11.960	12.010	12.145
ε_2	\nearrow	9.690	9.863	10.299	12.744

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: \nearrow and \searrow , noting that both η_p and E_{gp1} decrease with increasing T.

T in K	\nearrow	20	50	100	300

x=0					

For $r_a = r_{Ga}$,					
$\eta_p \gg 1$	\searrow	843	337	168	56
E_{gp1} in eV	\searrow	1.292	1.288	1.276	1.197
n	\nearrow	4.606	4.610	4.621	4.691
κ	\nearrow	2.697	2.709	2.745	2.975
ε_1	\searrow	13.941	13.910	13.820	13.156
ε_2	\nearrow	24.846	24.981	25.370	27.916

For $r_a = r_{In}$,

$\eta_p \gg 1$	↘	841	336.6	168	56
E_{gp1} in eV	↘	1.356	1.353	1.340	1.261
n	↗	4.448	4.452	4.464	4.535
κ	↗	2.518	2.529	2.564	2.786
ε_1	↘	13.451	13.426	13.352	12.801
ε_2	↗	22.400	22.526	22.890	25.274

For $r_a = r_{Cd}$,

$\eta_p \gg 1$	↘	841	336.3	168	56
E_{gp1} in eV	↘	1.384	1.380	1.368	1.289
n	↗	4.380	4.384	4.395	4.467
κ	↗	2.443	2.455	2.489	2.708
ε_1	↘	13.214	13.191	13.124	12.618
ε_2	↗	21.402	21.525	21.878	24.195

x=0.5

For $r_a = r_{Ga}$,

$\eta_p \gg 1$	↘	455	182	91	30
E_{gp1} in eV	↘	1.492	1.485	1.466	1.362
n	↗	4.252	4.259	4.276	4.372
κ	↗	2.163	2.181	2.229	2.503
ε_1	↘	13.404	13.382	13.320	12.846
ε_2	↗	18.395	18.579	19.062	21.888

For $r_a = r_{In}$,

$\eta_p \gg 1$	↘	452	181	90	30
E_{gp1} in eV	↘	1.530	1.523	1.504	1.400
n	↗	4.125	4.132	4.149	4.245
κ	↗	2.067	2.085	2.132	2.400
ε_1	↘	12.741	12.720	12.671	12.261
ε_2	↗	17.055	17.231	17.689	20.381

For $r_a = r_{Cd}$,

$\eta_p \gg 1$	↘	450	180	90	30
E_{gp1} in eV	↘	1.546	1.539	1.520	1.417
n	↗	4.069	4.076	4.094	4.190
κ	↗	2.027	2.045	2.091	2.357
ε_1	↘	12.449	12.433	12.385	12.000
ε_2	↗	16.499	16.671	17.119	19.754

x=1

For $r_a = r_{Ga}$,

$\eta_p \gg 1$	↘	310	124	62	20.65
E_{gp1} in eV	↘	1.956	1.946	1.921	1.793
n	↗	3.613	3.623	3.648	3.776
κ	↗	1.148	1.166	1.213	1.468
ε_1	↗	11.735	11.766	11.837	12.106
ε_2	↗	8.293	8.451	8.848	11.090

For $r_a = r_{In}$,

$\eta_p \gg 1$	↘	303	124	61	20.2
E_{gp1} in eV	↘	1.979	1.969	1.944	1.816
n	↗	3.505	3.516	3.541	3.670
κ	↗	1.105	1.123	1.169	1.420
ε_1	↗	11.068	11.099	11.172	11.453
ε_2	↗	7.748	7.898	8.277	10.423

For $r_a = r_{Cd}$,

$\eta_p \gg 1$	↘	299.7	120	60	19.94
E_{gp1} in eV	↘	1.989	1.979	1.954	1.826
n	↗	3.459	3.469	3.494	3.624
κ	↗	1.087	1.105	1.151	1.400
ε_1	↗	10.781	10.813	10.886	11.171

ε_2	\nearrow	7.523	7.671	8.042	10.147
-----------------	------------	-------	-------	-------	--------

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