



**OPTICAL COEFFICIENTS IN THE N(P)-TYPE DEGENERATE
GaSb(1-x) As(x)-CRYSTALLINE ALLOY, DUE TO THE NEW STATIC
DIELECTRIC CONSTANT-LAW AND THE GENERALIZED MOTT
CRITERIUM IN THE METAL-INSULATOR TRANSITION (12)**

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 20/09/2024

Article Revised on 10/10/2024

Article Accepted on 30/10/2024



***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 $\text{GaSb}_{1-x}\text{As}_x$ - 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 2.9×10^{-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}As_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 $X(x) \equiv \text{GaSb}_{1-x}\text{As}_x$ - 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:

$$E_{do(ao)}(x) = \frac{13600 \times [m_c(v)(x)/m_0]}{[\epsilon_0(x)]^2} \text{ meV}, \tag{4}$$

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 , $p_0 = 0$, and for the deformation potential energy (or the strain energy) σ , $\sigma_0 = 0$. Further, the two important equations^[1,7], used to determine the σ -variation, $\Delta\sigma \equiv \sigma - \sigma_0 = \sigma$, are defined by:

$\frac{dp}{dV} = -\frac{B}{V}$ and $p = -\frac{d\sigma}{dV}$. giving: $\frac{d}{dV}\left(\frac{d\sigma}{dV}\right) = \frac{B}{V}$. Then, by an integration, one gets:

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

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

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

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

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

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,

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

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,

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

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:

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

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 2.9×10^{-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 $m_r(x)/m_o$ 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:

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

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:

$$\Delta E_{\text{gno}}(N, r_d, x) = a_1 \times \frac{\varepsilon_0(x)}{\varepsilon(r_d, x)} \times N_r^{1/3} + a_2 \times \frac{\varepsilon_0(x)}{\varepsilon(r_d, x)} \times N_r^{1/3} \times (2.503 \times [-E_{\text{cn}}(r_{\text{sn}}) \times r_{\text{sn}}]) +$$

$$a_3 \times \left[\frac{\varepsilon_0(x)}{\varepsilon(r_d, x)} \right]^{5/4} \times \sqrt{\frac{m_v}{m_r}} \times N_r^{1/4} + a_4 \times \sqrt{\frac{\varepsilon_0(x)}{\varepsilon(r_d, x)}} \times N_r^{1/2} \times 2 + a_5 \times \left[\frac{\varepsilon_0(x)}{\varepsilon(r_d, x)} \right]^2 \times N_r^{1/6}$$

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

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

where $a_1 = 3.8 \times 10^{-3}$ (eV), $a_2 = 6.5 \times 10^{-4}$ (eV), $a_3 = 2.8 \times 10^{-3}$ (eV),

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

$$\Delta E_{\text{gpo}}(N, r_a, x) = a_1 \times \frac{\varepsilon_0(x)}{\varepsilon(r_a, x)} \times N_r^{1/3} + a_2 \times \frac{\varepsilon_0(x)}{\varepsilon(r_a, x)} \times N_r^{1/3} \times (2.503 \times [-E_{\text{cp}}(r_{\text{sp}}) \times r_{\text{sp}}]) +$$

$$a_3 \times \left[\frac{\varepsilon_0(x)}{\varepsilon(r_a, x)} \right]^{5/4} \times \sqrt{\frac{m_c}{m_r}} \times N_r^{1/4} + 2a_4 \times \sqrt{\frac{\varepsilon_0(x)}{\varepsilon(r_a, x)}} \times N_r^{1/2} + a_5 \times \left[\frac{\varepsilon_0(x)}{\varepsilon(r_a, x)} \right]^2 \times N_r^{1/6}$$

$$, N_r \equiv \left(\frac{N^*}{N_{\text{CDp}}(r_a, x)} \right), \Delta E_{\text{gp}}(N, r_a, x) = \Delta E_{\text{gpo}}(N, r_a, x) \times \{5 \times x + 8 \times (1 - x)\}, \quad (14p)$$

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

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

OPTICAL BAND GAP

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

$$E_{\text{gn1(gp1)}}(N, r_{d(a)}, x, T) \equiv$$

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

where $E_{\text{gn(gp)}}$, $[+E_{\text{Fn}}, -E_{\text{Fp}}] \geq 0$, 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:

$$E_{\text{gn1(gp1)}}(r_{d(a)}, x) = E_{\text{gno(gpo)}}(r_{d(a)}, x), \quad \text{according to: } N = N_{\text{CDn(NDp)}}(r_{d(a)}, x).$$

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 $\epsilon_2 \equiv 2n\kappa$. One notes that the optical absorption coefficient α is related to ϵ_2 , n , κ , and the optical conductivity σ_0 , by^[2]

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

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

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

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

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

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

Then, one has:

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

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

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

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

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:

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

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

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,

$$n(E, N, r_{d(a)}, x, T) = n_\infty(r_{d(a)}, x) + \sum_{i=1}^4 \frac{X_i(E_{gn1(gp1)}) \times E + Y_i(E_{gn1(gp1)})}{E^2 - B_i E + C_i}. \tag{21}$$

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:

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

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

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 $\mathbf{X(x)} \equiv \mathbf{GaSb}_{1-x}\mathbf{As}_x$ - 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:

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

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

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.

E. 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 $X(x) \equiv \text{GaSb}_{1-x}\text{As}_x$ - 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 2.9×10^{-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	1164	1164.97	1165	1165.03
n_{MIT}	\searrow	3.937	3.739	3.735	3.731
$\epsilon_{1(MIT)}$	\searrow	15.50	13.98	13.95	13.92
R_{MIT}	\searrow	0.354	0.334	0.33367	0.33324
-----At $x=1$,					
E_{CPE} in meV	\nearrow	1518.44	1519.96	1520	1520.04
n_{MIT}	\searrow	3.609	3.420	3.416	3.412
$\epsilon_{1(MIT)}$	\searrow	13.02	11.70	11.67	11.64
R_{MIT}	\searrow	0.320	0.300	0.2993	0.29888
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

$\varepsilon_{1(MIT)}$	↘	23.75	16.40	15.60	15.24
R_{MIT}	↘	0.435	0.365	0.355	0.351
<hr/>					
At $x=0.5$,					
E_{CPE} in meV	↗	1151.26	1165	1169	1171
n_{MIT}	↘	4.526	3.735	3.638	3.595
$\varepsilon_{1(MIT)}$	↘	20.49	13.95	13.23	12.92
R_{MIT}	↘	0.407	0.334	0.323	0.319
<hr/>					
At $x=1$,					
E_{CPE} in meV	↗	1503.7	1520	1524	1527
n_{MIT}	↘	4.173	3.416	3.323	3.281
$\varepsilon_{1(MIT)}$	↘	17.41	11.67	11.04	10.77
R_{MIT}	↘	0.376	0.299	0.289	0.284

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

Donor		P	Te	Sb	Sn
<hr/>					
At $x=0$,					
n_{∞}	↘	2.4604	2.2551	2.2507	2.2463
$\varepsilon_{1,\infty}$	↘	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
<hr/>					
At $x=0.5$,					
n_{∞}	↘	2.3579	2.1611	2.1570	2.1527
$\varepsilon_{1,\infty}$	↘	5.5597	4.6704	4.6525	4.6342
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	10.7593	9.8614	9.8424	9.8230

α_{∞} in $(10^9 \times cm^{-1})= 2.1602$

$R_{\infty} \searrow$ 0.1635 0.1349 0.1343 0.1337

At $x=1$,

$n_{\infty} \searrow$ 2.2507 2.0629 2.0589 2.0549

$\epsilon_{1,\infty} \searrow$ 5.0658 4.2556 4.2392 4.2226

$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm} \searrow$ 10.2703 9.4132 9.3951 9.3766

α_{∞} in $(10^9 \times cm^{-1})= 2.1602$

$R_{\infty} \searrow$ 0.1480 0.1204 0.1198 0.1192

Acceptor

B

Ga

In

Cd

At $x=0$,

$n_{\infty} \searrow$ 3.067 2.251 2.152 2.108

$\epsilon_{1,\infty} \searrow$ 9.407 5.066 4.629 4.444

$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm} \searrow$ 13.99 10.27 9.818 9.619

α_{∞} in $(10^9 \times cm^{-1})= 2.1602$

$R_{\infty} \searrow$ 0.258 0.148 0.133 0.127

At $x=0.5$,

$n_{\infty} \searrow$ 2.939 2.157 2.062 2.020

$\epsilon_{1,\infty} \searrow$ 8.639 4.652 4.252 4.081

$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm} \searrow$ 13.41 9.842 9.409 9.218

α_{∞} in $(10^9 \times cm^{-1})= 2.1602$

$R_{\infty} \searrow$ 0.242 0.134 0.120 0.114

At $x=1$,

$n_{\infty} \searrow$ 2.806 2.059 1.968 1.928

$\epsilon_{1,\infty} \searrow$ 7.872 4.239 3.874 3.719

$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm} \searrow$ 12.80 9.395 8.981 8.799

α_{∞} in $(10^9 \times cm^{-1})= 2.1602$

$R_{\infty} \searrow$ 0.225 0.120 0.106 0.100

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,				
$E_{CPE} = 1.1639$	3.9370	0	15.4999	0
2	4.721	0.196	22.255	1.855
2.5	5.605	0.676	30.958	7.576
3	5.329	2.769	20.727	29.514
3.5	4.008	2.842	7.990	22.780
4	4.186	2.435	11.597	20.384
4.5	4.623	3.622	8.255	33.486
5	2.459	4.919	-18.150	24.195
5.5	1.044	3.401	-10.474	7.101
6	1.243	2.493	-4.670	6.200
...				
10^{22}	2.3579	0	5.5597	0

At x=1,

$E_{CPE} = 1.5184$	3.6089	0	13.0242	0
2	3.996	0.222	15.922	1.775
2.5	4.671	0.365	21.688	3.408
3	4.693	1.803	18.777	16.925
3.5	3.847	2.045	10.623	15.733
4	3.993	1.864	12.470	14.886
4.5	4.354	2.893	10.591	25.192
5	2.592	4.052	-9.698	21.006
5.5	1.373	2.867	-6.337	7.871
6	1.500	2.141	-2.333	6.425
...				
10^{22}	2.2507	0	5.0658	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} =1.1512 4.5262 0 20.4868 0

2	5.327	0.195	28.336	2.074
2.5	6.218	0.689	38.187	8.564
3	5.929	2.807	27.275	33.293
3.5	4.590	2.872	12.819	26.371
4	4.770	2.456	16.717	23.433
4.5	5.209	3.649	13.823	38.021
5	3.031	4.951	-15.332	30.015
5.5	1.608	3.420	-9.112	11.004
6	1.810	2.506	-3.003	9.075
...				

10²² 2.9393 0 8.6393 0

At $x=1$,

E_{CPE} =1.5537 4.1730 0 17.4142 0

2	4.575	0.222	20.883	2.033
2.5	5.258	0.376	27.509	3.952
3	5.270	1.839	24.390	19.384
3.5	4.406	2.075	15.106	18.286
4	4.552	1.886	17.168	17.174
4.5	4.916	2.921	15.638	28.727
5	3.138	4.086	-6.847	25.649
5.5	1.911	2.888	-4.692	11.040
6	2.041	2.155	-0.477	8.799
...				

10²² 2.8057 0 7.8719 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.

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	188.7	329	463
E_{gn1} in eV	↗	1.070	1.076	1.117	1.178
n	↘	4.707	4.702	4.667	4.614
κ	↘	3.362	3.344	3.215	3.030
ϵ_1	↗	10.855	10.928	11.442	12.104
ϵ_2	↘	31.652	31.454	30.005	27.961

For $r_d = r_{Sn}$,

$\eta_n \gg 1$	↗	131	188.7	329	463
E_{gn1} in eV	↗	1.071	1.077	1.120	1.181
n	↘	4.702	4.697	4.660	4.607
κ	↘	3.359	3.340	3.208	3.022
ε_1	↗	10.829	10.906	11.428	12.093
ε_2	↘	31.586	31.376	29.902	27.846

x=1

For $r_d = r_{Sb}$,

$\eta_n \gg 1$	↗	93	135	236	332
E_{gn1} in eV	↗	1.456	1.462	1.496	1.543
n	↘	4.265	4.260	4.228	4.184
κ	↘	2.256	2.240	2.153	2.036
ε_1	↗	13.105	13.127	13.240	13.359
ε_2	↘	19.242	19.087	18.210	17.052

For $r_d = r_{Sn}$,

$\eta_n \gg 1$	↗	93.6	135	236	332
E_{gn1} in eV	↗	1.456	1.462	1.497	1.545
n	↘	4.261	4.255	4.223	4.178
κ	↘	2.254	2.238	2.150	2.031
ε_1	↗	13.074	13.096	13.210	13.330
ε_2	↘	19.204	19.043	18.156	16.972

$N (10^{18} \text{ cm}^{-3})$	↗	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 $r_a = r_{Ga}$,

$\eta_p \gg 1$	↗	125	184	326	460
E_{gp1} in eV	↗	1.079	1.093	1.157	1.238
n	↘	4.700	4.687	4.632	4.561
κ	↘	3.334	3.289	3.094	2.854
ε_1	↗	10.971	11.152	11.884	12.659
ε_2	↘	31.336	30.836	28.669	26.032

For $r_a = r_{In}$,

$\eta_p \gg 1$	↗	123.8	183	325.2	459.6
E_{gp1} in eV	↗	1.099	1.119	1.195	1.286
n	↘	4.587	4.570	4.504	4.423
κ	↘	3.272	3.210	2.981	2.714
ε_1	↗	10.340	10.583	11.403	12.193
ε_2	↘	30.021	29.344	26.851	24.008

For $r_a = r_{Cd}$,

$\eta_p \gg 1$	↗	123	182.1	324.6	459.1
E_{gp1} in eV	↗	1.108	1.130	1.211	1.307
n	↘	4.538	4.519	4.448	4.362
κ	↘	3.245	3.176	2.932	2.655
ε_1	↗	10.064	10.331	11.185	11.977
ε_2	↘	29.458	28.710	26.088	23.168

x=1

For $r_a = r_{Ga}$,

$\eta_p \gg 1$	↗	89	131	233	329
E_{gp1} in eV	↗	1.462	1.474	1.524	1.586

n	\searrow	4.259	4.248	4.201	4.143
κ	\searrow	2.238	2.207	2.082	1.931
ε_1	\nearrow	13.130	13.173	13.317	13.434
ε_2	\searrow	19.067	18.751	17.491	15.996

For $r_a = r_{In}$,

$\eta_p \gg 1$	\nearrow	87	130	232	328.6
E_{gp1} in eV	\nearrow	1.477	1.493	1.552	1.621

n	\searrow	4.154	4.139	4.085	4.019
κ	\searrow	2.200	2.159	2.014	1.848
ε_1	\nearrow	12.421	12.474	12.629	12.735
ε_2	\searrow	18.277	17.875	16.453	14.857

For $r_a = r_{Cd}$,

$\eta_p \gg 1$	\nearrow	86.5	129.2	231.7	328.2
E_{gp1} in eV	\nearrow	1.484	1.502	1.564	1.636

n	\searrow	4.108	4.092	4.033	3.964
κ	\searrow	2.183	2.138	1.985	1.813
ε_1	\nearrow	12.114	12.172	12.329	12.429
ε_2	\searrow	17.936	17.498	16.014	14.380

N (10^{18} 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 η_n ($\gg 1$, 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	1.178	1.171	1.152	1.049
n	\nearrow	4.614	4.620	4.636	4.726
κ	\nearrow	3.030	3.052	3.108	3.431
ε_1	\searrow	12.104	12.031	11.836	10.563
ε_2	\nearrow	27.961	27.199	28.819	32.427

For $r_d = r_{Sn}$,

$\eta_n \gg 1$	\searrow	463	185	92.6	31
E_{gn1} in eV	\searrow	1.181	1.174	1.155	1.051
n	\nearrow	4.607	4.613	4.630	4.719
κ	\nearrow	3.022	3.044	3.099	3.422
ε_1	\searrow	12.093	12.020	11.826	10.560
ε_2	\nearrow	27.846	28.083	28.702	32.300

x=1

For $r_d = r_{Sb}$,

$\eta_n \gg 1$	\searrow	332	133	66	22
E_{gn1} in eV	\searrow	1.543	1.533	1.508	1.380
n	\nearrow	4.184	4.193	4.216	4.335
κ	\nearrow	2.036	2.060	2.122	2.456
ε_1	\searrow	13.359	13.338	13.275	12.762
ε_2	\nearrow	17.035	17.280	17.895	21.295

For $r_d = r_{Sn}$,

$\eta_n \gg 1$	\searrow	332	133	66	22
E_{gn1} in eV	\searrow	1.545	1.535	1.510	1.382
n	\nearrow	4.178	4.187	4.211	4.329
κ	\nearrow	2.031	2.056	2.117	2.451
ε_1	\searrow	13.330	13.308	13.246	12.737
ε_2	\nearrow	16.973	17.217	17.830	21.223

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 $r_a = r_{In}$,

$\eta_p \gg 1$	\searrow	841	336.6	168	56
E_{gp1} in eV	\searrow	1.356	1.353	1.340	1.261

n	\nearrow	4.448	4.452	4.464	4.535
κ	\nearrow	2.518	2.529	2.564	2.786
ε_1	\searrow	13.451	13.426	13.352	12.801
ε_2	\nearrow	22.400	22.526	22.890	25.274

For $r_a = r_{Cd}$,

$\eta_p \gg 1$	\searrow	841	336.3	168	56
E_{gp1} in eV	\searrow	1.384	1.380	1.368	1.289

n	\nearrow	4.380	4.384	4.395	4.467
κ	\nearrow	2.443	2.455	2.489	2.708
ε_1	\searrow	13.214	13.191	13.124	12.618
ε_2	\nearrow	21.402	21.525	21.878	24.195

x=0.5

For $r_a = r_{Ga}$,

$\eta_p \gg 1$	\searrow	460	184	92	31
E_{gp1} in eV	\searrow	1.238	1.231	1.212	1.108

n	\nearrow	4.561	4.567	4.584	4.674
κ	\nearrow	2.854	2.875	2.929	3.243
ε_1	\searrow	12.659	12.597	12.431	11.335
ε_2	\nearrow	26.032	26.259	26.854	30.317

For $r_a = r_{In}$,

$\eta_p \gg 1$	↘	459.6	184	92	30.6
E_{gp1} in eV	↘	1.286	1.279	1.261	1.157
n	↗	4.423	4.429	4.446	4.537
κ	↗	2.714	2.735	2.788	3.094
ε_1	↘	12.193	12.139	11.993	11.014
ε_2	↗	24.008	24.224	24.788	28.077

For $r_a = r_{Cd}$,

$\eta_p \gg 1$	↘	459.1	183.6	91.8	30.6
E_{gp1} in eV	↘	1.307	1.300	1.281	1.178
n	↗	4.362	4.369	4.385	4.577
κ	↗	2.655	2.676	2.728	3.031
ε_1	↘	11.977	11.925	11.787	10.857
ε_2	↗	23.168	23.379	23.930	27.145

x=1

For $r_a = r_{Ga}$,

$\eta_p \gg 1$	↘	329	132	66	22
E_{gp1} in eV	↘	1.586	1.576	1.551	1.423
n	↗	4.143	4.152	4.176	4.295
κ	↗	1.931	1.955	2.015	2.340
ε_1	↘	13.434	13.420	13.377	12.973
ε_2	↗	15.996	16.232	16.824	20.106

For $r_a = r_{In}$,

$\eta_p \gg 1$	↘	328.6	131	66	22
E_{gp1} in eV	↘	1.621	1.611	1.586	1.458
n	↗	4.019	4.028	4.052	4.173
κ	↗	1.848	1.872	1.931	2.250
ε_1	↘	12.735	12.724	12.692	12.349
ε_2	↗	14.857	15.082	15.646	18.775

For $r_a = r_{Cd}$,

$\eta_p \gg 1$ \searrow 328.2 131 65.6 21.8

E_{gp1} in eV \searrow 1.636 1.626 1.601 1.473

n \nearrow 3.964 3.974 3.998 4.119

κ \nearrow 1.813 1.837 1.895 2.211

ϵ_1 \searrow 12.429 12.420 12.392 12.075

ϵ_2 \nearrow 14.380 14.599 15.151 18.215

T in K \nearrow 20 50 100 300
