wjert, 2024, Vol. 10 Issue 10, 180-204. *Original Article* **ISSN 2454-695X**

World Journal of Engineering Research and Technology
WJERT

www.wjert.org **SJIF Impact Factor: 7.029**

OPTICAL COEFFICIENTS IN THE N(P)-TYPE DEGENERATE GaAs(1-x) Sb(x)-CRYSTALLINE ALLOY, DUE TO THE NEW STATIC DIELECTRIC CONSTANT-LAW AND THE GENERALIZED MOTT CRITERIUM IN THE METAL-INSULATOR TRANSITION. (2)

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Article Received on 16/08/2024 **Article Revised on 06/09/2024** **Article Accepted on 26/09/2024**

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ABTRACT

In the n(p)-type $GaAs_{1-x}Sb_x$- crystalline alloy, with $0 \leq x \leq 1$, basing on our two recent works[1,2], for a given x, and with an increasing $r_{d(a)}$, the optical coefficients have been determined, as functions of the photon energy E, total impurity density N, the donor (acceptor) radius $r_{d(a)}$, concentration x, and temperature T. Those results have been affected by **(i)** the important new $\varepsilon(r_{d(a)}, x)$-law, developed in Equations (8a, 8b), stating that, for a given x, due to the impurity-size effect, ε decreases (↘) with an increasing (↗) $r_{d(a)}$, and then by **(ii)** the generalized Mott critical d(a)-density defined in the metal-insulator transition (MIT), $N_{CDn(NDp)}(r_{d(a)}, x)$, as observed in Equations (8c, 9a). Furthermore, we also showed that $N_{CDn(NDp)}$ is just the density of carriers localized in exponential band tails, with a precision of the order of 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.

KEYWORS: $GaAs_{1-x}Sb_x$- 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 $X(x) \equiv GaAs_{1-x}Sb_x$ - crystalline alloy, with $0 \leq x \leq 1$, are investigated, as functions of the photon energy E, total impurity density N, the donor (acceptor) radius $r_{d(a)}$, concentration x, and temperature T.

Then, for a given x, and with an increasing $r_{d(a)}$, the numerical results of all the optical coefficients, obtained in appropriated physical conditions (E, N, T), and calculated by using Equations (15, 16, 20, 21), are reported in Tables 1, 2, 3n, 3p, 4n, 4p, 5n, and 5p in Appendix 1.

ENERGY BAND STUCTURE PARAMETERS

First of all, in the $n^+(p^+) - p(n)\ X(x)$- crystalline alloy at T=0 K, we denote the donor (acceptor) d(a)- radius by $r_{d(a)}$, and also the intrinsic one by: $r_{do(ao)}$=$r_{As(Ga)}$=0.118 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:

$$m_{c(v)}(x)/m_o = 0.047(0.3) \times x + 0.066\ (0.291) \times (1-x) \qquad (1)$$

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

$$\varepsilon_o(x) = 15.69 \times x + 13.13 \times (1-x). \qquad (2)$$

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

$$E_{go}(x) = 0.81 \times x + 1.52 \times (1-x). \qquad (3)$$

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

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

and then, the isothermal bulk modulus, by:

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

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

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

At $r_{d(a)} = r_{do(ao)}$, the needed boundary conditions are found to be, for the impurity-atom volume V= $(4\pi/3) \times \left(r_{d(a)}\right)^3$, $V_{do(ao)} = (4\pi/3) \times \left(r_{do(ao)}\right)^3$, for the pressure p, $p_o = 0$, and for the deformation potential energy (or the strain energy) σ, $\sigma_o = 0$. Further, the two important equations[1,7], used to determine the σ-variation, $\Delta\sigma \equiv \sigma - \sigma_o = \sigma$, are defined by: $\frac{dp}{dV} = -\frac{B}{V}$ and $p = -\frac{d\sigma}{dV}$. giving: $\frac{d}{dV}\left(\frac{d\sigma}{dV}\right) = \frac{B}{V}$. Then, by an integration, one gets:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

depending thus on our **new $\varepsilon(r_{d(a)},x)$-law.**

This excellent one can be explained from the definition of the reduced effective Wigner-Seitz (**WS**) radius $r_{sn(sp)}$, characteristic of interactions, by:

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

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

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

Thus, the above Equations (9a, 9b, 9c) confirm our new $\varepsilon(r_{d(a)},x)$-law, given in Equations (8a, 8b). Furthermore, by using $\mathbf{M_{n(p)} = 0.25}$, according to the empirical Heisenberg parameter $\mathcal{H}_{n(p)} = \mathbf{0.47137}$, as those given in Equations (8, 15) of the Ref. [1], we have also showed that $N_{CDn(CDp)}$ is just the density of electrons (holes) localized in the exponential conduction (valence)-band tail, with a precision of the order of $\mathbf{2.9 \times 10^{-7}}$. Therefore, the density of electrons (holes) given in parabolic conduction (valence) bands can be defined, as that given in compensated materials, by:

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

$$E_{gni(gpi)}(r_{d(a)}, x, T) \text{ in eV} = E_{gno(gpo)}(r_{d(a)}, x) - 10^{-4} \times T^2 \times \left\{\frac{7.205 \times x}{T+94\ K} + \frac{5.405 \times (1-x)}{T+204\ K}\right\}, \quad (10)$$

suggesting that, for given x and $r_{d(a)}$, $E_{gni(gpi)}$ decreases with an increasing T.

Then, in the following, for the study of optical phenomena, one denote the conduction (valence)-band density of states by $N_{c(v)}(T,x)$ as:

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

where $m_r(x)/m_c$ is the reduced effective mass $m_r(x)/m_c$, defined by :

$m_r(x) \equiv [m_c(x) \times m_v(x)]/[m_c(x) + m_v(x)]$.

D. Heavy Doping Effect, with given T, x and $r_{d(a)}$

Here, as given in our previous works[1,2], the Fermi energy $E_{Fn}(-E_{Fp})$, and the band gap narrowing are reported in the following.

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

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

where u is the reduced electron density, $u(N, r_{d(a)}, x, T) \equiv \frac{N^*}{N_{c(v)}(T,x)}$, $F(u) = au^{\frac{2}{3}}\left(1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}}\right)^{-\frac{2}{3}}$,

$a = [(3\sqrt{\pi}/4) \times u]^{2/3}$, $b = \frac{1}{8}\left(\frac{\pi}{a}\right)^2$, $c = \frac{62.3739855}{1920}\left(\frac{\pi}{a}\right)^4$, and $G(u) \simeq Ln(u) + 2^{-\frac{3}{2}} \times u \times e^{-du}$;

$d = 2^{3/2}\left[\frac{1}{\sqrt{27}} - \frac{3}{16}\right] > 0$. Therefore, from Eq. (12), the Fermi energies are expressed as functions of variables: $N, r_{d(a)}, x$, and T.

Here, one notes that: (i) as $u \gg 1$, according to the HD [d(a)- X(x)- alloy] ER-case, or to the degenerate case, Eq. (12) is reduced to the function F(u), and in particular at T=0 and as

$N^* = 0$, according to the metal- insulator transition (**MIT**), one has: $+E_{Fn}(-E_{Fp}) = \frac{\hbar^2}{2\times m_r(x)} \times (3\pi^2 N^*)^{2/3} = 0$, and (ii) $\frac{E_{Fn}(u\ll1)}{k_BT}\left(\frac{-E_{Fp}(u\ll1)}{k_BT}\right) \ll -1$, 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:

$$r_{sn(sp)}(N, r_{d(a)}, x) = 1.1723 \times 10^8 \times \left(\frac{g_{c(v)}(x)}{N^*}\right)^{1/3} \times \frac{m_r(x)}{\varepsilon(r_{d(a)}, x)}, \qquad (13a)$$

the correlation energy of an effective electron gas, $E_{cn(cp)}(N, r_{d(a)}, x)$, is given as:

$$E_{cn(cp)}(N, r_{d(a)}, x) = \frac{-0.87553}{0.0908 + r_{sn(sp)}} + \frac{\frac{0.87553}{0.0908 + r_{sn(sp)}} + \left(\frac{2[1-\ln(2)]}{\pi^2}\right) \times \ln(r_{sn(sp)}) - 0.093288}{1 + 0.03847728 \times r_{sn(sp)}^{1.67378876}}. \qquad (13b)$$

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:

$$\Delta E_{gn}(N, r_d, x) \simeq a_1 \times \frac{\varepsilon_0(x)}{\varepsilon(r_d, x)} \times N_r^{1/3} + a_2 \times \frac{\varepsilon_0(x)}{\varepsilon(r_d, x)} \times N_r^{\frac{1}{3}} \times (2.503 \times [-E_{cn}(r_{sn}) \times r_{sn}]) + a_3 \times \left[\frac{\varepsilon_0(x)}{\varepsilon(r_d, x)}\right]^{5/4} \times \sqrt{\frac{m_v}{m_r}} \times N_r^{1/4} + a_4 \times \sqrt{\frac{\varepsilon_0(x)}{\varepsilon(r_d, x)}} \times N_r^{1/2} \times 2 + a_5 \times \left[\frac{\varepsilon_0(x)}{\varepsilon(r_d, x)}\right]^{\frac{3}{2}} \times N_r^{\frac{1}{6}}, \quad N_r \equiv \left(\frac{N^*}{N_{CDn}(r_d, x)}\right), \qquad (14n)$$

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:

$$\Delta E_{gp}(N, r_a, x) \simeq a_1 \times \frac{\varepsilon_0(x)}{\varepsilon(r_a, x)} \times N_r^{1/3} + a_2 \times \frac{\varepsilon_0(x)}{\varepsilon(r_a, x)} \times N_r^{\frac{1}{3}} \times (2.503 \times [-E_{cp}(r_{sp}) \times r_{sp}]) + a_3 \times \left[\frac{\varepsilon_0(x)}{\varepsilon(r_a, x)}\right]^{5/4} \times \sqrt{\frac{m_c}{m_r}} \times N_r^{1/4} + 2a_4 \times \sqrt{\frac{\varepsilon_0(x)}{\varepsilon(r_a, x)}} \times N_r^{1/2} + a_5 \times \left[\frac{\varepsilon_0(x)}{\varepsilon(r_a, x)}\right]^{\frac{3}{2}} \times N_r^{\frac{1}{6}}, \quad N_r \equiv \left(\frac{N^*}{N_{CDp}(r_a, x)}\right), \qquad (14p)$$

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

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

OPTICAL BAND GAP

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

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

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

OPTICAL COEFFICIENTS

The optical properties of any medium can be described by the complex refraction index $\mathbb{N}$ and the complex dielectric function ε, $\mathbb{N} \equiv n - i\kappa$ and $\varepsilon \equiv \varepsilon_1 - i\varepsilon_2$, where $i^2 = -1$ and $\varepsilon \equiv \mathbb{N}^2$. Therefore, the real and imaginary parts of ε denoted by ε_1 and ε_2 can thus be expressed in terms of the refraction index n and the extinction coefficient κ as: $\varepsilon_1 \equiv n^2 - \kappa^2$ and $\varepsilon_2 \equiv 2n\kappa$. One notes that the optical absorption coefficient α is related to ε_2, n, κ, and the optical conductivity σ_O, by[2]

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

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

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

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

From Equations (16, 17), if the two optical functions, ε_1 and ε_2, (or n and κ), are both known, the other ones defined above can thus be determined, noting also that:

$\mathbf{E_{gn1(gp1)}(N, r_{d(a)}, x, T) = E_{gn1(gp1)}}$, for a presentation simplicity.

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

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

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

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

Further, one notes that, as $E \to \infty$, Forouhi and Bloomer (FB)[4] claimed that $\kappa(E \to \infty) \to$ a constant, while the $\kappa(E)$ -expressions, proposed by Van Cong[2] quickly go to 0 as E^{-3}, and consequently, their numerical results of the optical functions such as: $\sigma_O(E)$ and $\alpha(E)$, given in Eq. (16), both go to 0 as E^{-2}.

Now, an improved Forouhi-Bloomer parameterization model (FB-PM), used to determine the expressions of the optical coefficients in the degenerate $n^+(p^+) - p(n)\ X(x)$- crystalline alloy, is now proposed as follows. Then, if denoting the functions G(E) and F(E) and by: $G(E) \equiv \sum_{i=1}^{4} \frac{A_i}{E^2 - B_i E + C_i}$ and $F(E) \equiv \sum_{i=1}^{4} \frac{A_i}{E^2 \times (1 + 10^{-4} \times \frac{E}{6}) - B_i E + C_i}$, we propose:

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

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

being equal to 0 for $E^* = 0$ (or for $E = E_{gn1(gp1)}$), and also going to 0 as E^{-1} as $E \to \infty$, and further, $n(E, N, r_{d(a)}, x, T) = n_\infty(r_{d(a)}, x) + \sum_{i=1}^{4} \frac{X_i(E_{gn1(gp1)}) \times E + Y_i(E_{gn1(gp1)})}{E^2 - B_i E + C_i}$ (21)

going to a constant as $E \to \infty$, since $n(E \to \infty, r_{d(a)}, x) \to n_\infty(r_{d(a)}, x) = \sqrt{\varepsilon(r_{d(a)}, x)} \times \frac{\omega_T}{\omega_L}$, $\omega_L = 8.9755 \times 10^{13}\ s^{-1}$ [5] and $\omega_L = 8.9755 \times 10^{13}\ s^{-1}$.

Here, the other parameters are determined by: $X_i(E_{gn1(gp1)}) = \frac{A_i}{Q_i} \times \left[-\frac{B_i^2}{2} + E_{gn1(gp1)} B_i - E_{gn1(gp1)}^2 + C_i\right]$,

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

$A_i = 1.154 \times A_{i(FB)} = 4.7314 \times 10^{-4}$, 0.2314, 0.1118 and 0.0116 ,

$B_i \equiv B_{i(FB)} = 5.871, 6.154, 9.679$ and 13.232, and $C_i \equiv C_{i(FB)} = 8.619, 9.784, 23.803,$ and 44.119.

Then, as noted above, if the two optical functions, n and κ, are both known, the other ones defined in Equations (16, 17) can also be determined.

NUMERICAL RESULTS

Now, some numerical results of those optical functions are investigated in the n(p)-type $X(x) \equiv GaAs_{1-x}Sb_x$ crystalline alloy, as follows.

A. Metal-insulator transition (MIT)-case

As discussed above, the physical conditions used for the MIT are found to be given by: T=0K, $N^* = 0$ or $N = N_{CDn(CDp)}$, giving rise to: $E_{gn1(gp1)}(N^* = 0, r_{d(a)}, x, T = 0) = E_{gn1(gp1)}(r_{d(a)}, x) = E_{gno(gpo)}(r_{d(a)}, x)$.

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

B. Optical coefficients, obtained as E → ∞

In Eq. (21), at any T, the choice of the real refraction index: $n(E \to \infty, r_{d(a)}, x, T) = n_\infty(r_{d(a)},x) = \sqrt{\varepsilon(r_{d(a)},x)} \times \frac{\omega_T}{\omega_L}$, $\omega_T = 5.1 \times 10^{13}\, s^{-1}$[5] and $\omega_L = 8.9755 \times 10^{13}\, s^{-1}$, was obtained from the Lyddane-Sachs-Teller relation[5], from which T(L) represent the transverse (longitudinal) optical phonon modes. Then, from Equations (16, 17, 20), from such the asymptotic behavior ($E \to \infty$), we obtain: $\kappa_\infty(r_{d(a)},x) \to 0$ and $\varepsilon_{2,\infty}(r_{d(a)},x) \to 0$, as E^{-1}, so that $\varepsilon_{1,\infty}(r_{d(a)},x)$, $\sigma_{O,\infty}(r_{d(a)},x)$, $\alpha_\infty(r_{d(a)},x)$ and $R_\infty(r_{d(a)},x)$ go to their appropriate limiting constants, 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 $E\ [\geq E_{CPE}(r_{d(a)}, x)]$ and for given x, as those reported in Tables 3n and 3p in Appendix 1.

D. Variations of various optical coefficients, as functions of N

In the X(x)-system, at E=3.2 eV and T=20 K, for given $r_{d(a)}$ and x, and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of $\eta_{n(p)}(\gg 1, \text{degenerate case})$, $E_{gn1(gp1)}$, n, κ, ε_1 and ε_2, obtained as functions of N, being represented by the arrows: ↗ and ↘, as those tabulated in Tables 4n and 4p in Appendix 1.

E. Variations of various optical coefficients as functions of T

In the X(x)-system, at E=3.2 eV and $N = 10^{20}\,cm^{-3}$, for given $r_{d(a)}$ and x, and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of $\eta_{n(p)}(\gg 1, \text{degenerate case})$, $E_{gn1(gp1)}$, n, κ, ε_1 and ε_2, obtained as functions of T, being represented by the arrows: ↗ and ↘, as those tabulated in Tables 5n and 5p in Appendix 1.

CONCLUDING REMARKS

In the n(p)-type $X(x) \equiv GaAs_{1-x}Sb_x$- 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 $2.9\ \times 10^{-7}$, as that given in Table 4 of Ref.[1], according to a definition of the effective density of electrons (holes) given inparabolic 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.

ACKNOWLEDGMENT

The author is thankful to: M. Cayrol and J. Sulian for their technical dupport, and also P. Blaise, R. Brouzet and O. Henri-Rousseau for their encouragement, during the preparation of this work.

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APPENDIX 1

Table 1: In the MIT-case, T=0K, N= $N_{CDn(p)}(r_{d(a)}, x)$**, and the critical photon energy** $E_{CPE} = E = E_{gno(gpo)}(r_{d(a)}, x)$**, if** $E = E_{gn1(gp1)}(r_{d(a)}, x) = E_{CPE}(r_{d(a)}, x)$**, the numerical results of optical functions such as:** $n_{MIT}(r_{d(a)}, x)$**, obtained from Eq. (21), and those of other ones:** $\varepsilon_{1(MIT)}(r_{d(a)}, x)$ **and** $R_{MIT}(r_{d(a)}, x)$, from Eq. (16) **decrease (↘) with increasing (↗)** $r_{d(a)}$ **and** E_{CPE}

Donor		P	As	Te	Sb	Sn
r_d (nm) [4]	↗	0.110	0.118	0.132	0.136	0.140
At **x=0**,						
E_{CPE} in meV	↗	1519.8	1520	1520.7	1521.2	1521.8
n_{MIT}	↘	3.437	3.416	3.352	3.313	3.268
$\varepsilon_{1(MIT)}$	↘	11.81	11.67	11.23	10.98	10.68
R_{MIT}	↘	0.302	0.299	0.292	0.288	0.282
At **x=0.5**,						
E_{CPE} in meV	↗	1664.8	1665	1665.5	1665.8	1666.3
n_{MIT}	↘	3.446	3.424	3.356	3.316	3.269
$\varepsilon_{1(MIT)}$	↘	11.87	11.72	11.27	10.99	10.69
R_{MIT}	↘	0.303	0.300	0.292	0.288	0.282
At **x=1**,						
E_{CPE} in meV	↗	1809.9	1810	1810.3	1810.6	1810.9
n_{MIT}	↘	3.450	3.427	3.357	3.315	3.266
$\varepsilon_{1(MIT)}$	↘	11.90	11.74	11.27	10.99	10.67
R_{MIT}	↘	0.303	0.300	0.293	0.288	0.282

Acceptor		B	Ga	Mg	In	Cd
r_a (nm)	↗	0.088	0.126	0.140	0.144	0.148
At **x=0**,						
E_{CPE} in meV	↗	1503.7	1520	1523	1524	1527
n_{MIT}	↘	4.173	3.416	3.358	3.323	3.281
$\varepsilon_{1(MIT)}$	↘	17.41	11.67	11.276	11.04	10.77
R_{MIT}	↘	0.376	0.299	0.293	0.289	0.284

At x=0.5,						
E_{CPE} in meV	↗	1651	1665	1667	1669	1671
n_{MIT}	↘	4.215	3.424	3.363	3.326	3.283
$\varepsilon_{1(MIT)}$	↘	17.76	11.72	11.31	11.06	10.78
R_{MIT}	↘	0.380	0.300	0.293	0.289	0.284
At x=1,						
E_{CPE} in meV	↗	1798	1810	1812	1813	1815
n_{MIT}	↘	4.251	3.427	3.364	3.326	3.281
$\varepsilon_{1(MIT)}$	↘	18.07	11.74	11.32	11.06	10.77
R_{MIT}	↘	0.383	0.300	0.293	0.289	0.284

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

Donor		P	As	Te	Sb	Sn
At x=0,						
n_{∞}	↘	2.08	2.0589	1.9950	1.9566	1.9124
$\varepsilon_{1,\infty}$	↘	4.327	4.2392	3.9800	3.8284	3.6571
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	9.4915	9.3951	9.1033	8.9282	8.7263
α_{∞} in $(10^7 \times cm^{-1})$		2.160	2.160	2.160	2.160	2.160
R_{∞}	↘	0.123	0.120	0.110	0.105	0.098
At x=0.5,						
n_{∞}	↘	2.179	2.157	2.090	2.050	2.003
$\varepsilon_{1,\infty}$	↘	4.748	4.652	4.368	4.202	4.014
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	9.943	9.842	9.537	9.353	9.142
α_{∞} in $(10^7 \times cm^{-1})$		2.160	2.160	2.160	2.160	2.160
R_{∞}	↘	0.137	0.134	0.124	0.118	0.112

At **x=1**,					
n_∞ ↘	2.274	2.251	2.181	2.139	2.090
$\varepsilon_{1,\infty}$ ↘	5.170	5.066	4.756	4.575	4.370
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega\times cm}$ ↘	10.37	10.27	9.951	9.760	9.539
α_∞ in $(10^9\times cm^{-1})$	2.160	2.160	2.160	2.160	2.160
R_∞ ↘	0.151	0.148	0.138	0.132	0.124

Acceptor	B	Ga	Mg	In	Cd
At **x=0**,					
n_∞ ↘	2.806	2.059	2.002	1.968	1.928
$\varepsilon_{1,\infty}$ ↘	7.872	4.239	4.010	3.874	3.719
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega\times cm}$ ↘	12.80	9.395	9.138	8.981	8.799
α_∞ in $(10^9\times cm^{-1})$	2.160	2.160	2.160	2.160	2.160
R_∞ ↘	0.225	0.120	0.111	0.106	0.100
At **x=0.5**,					
n_∞ ↘	2.939	2.157	2.098	2.062	2.020
$\varepsilon_{1,\infty}$ ↘	8.639	4.652	4.401	4.252	4.081
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega\times cm}$ ↘	13.41	9.842	9.573	9.409	9.218
α_∞ in $(10^9\times cm^{-1})$	2.160	2.160	2.160	2.160	2.160
R_∞ ↘	0.242	0.134	0.125	0.120	0.114
At **x=1**,					
n_∞ ↘	3.067	2.251	2.189	2.152	2.108
$\varepsilon_{1,\infty}$ ↘	9.407	5.066	4.792	4.629	4.444
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega\times cm}$ ↘	13.99	10.27	9.989	9.818	9.619
α_∞ in $(10^9\times cm^{-1})$	2.160	2.160	2.160	2.160	2.160
R_∞ ↘	0.258	0.148	0.139	0.133	0.127

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) $\kappa = 0$

E in eV	n	κ	ε_1	ε_2
At x=0,				
$E_{CPE} = 1.5198$	**3.437**	**0**	**11.816**	**0**
1.6	3.489	0.055	12.172	0.508
2	3.823	0.222	14.570	1.698
2.5	4.498	0.364	20.097	3.272
3	4.521	1.800	17.197	16.272
3.5	3.676	2.042	9.347	15.013
4	3.822	1.862	11.140	14.232
4.5	4.183	2.890	9.143	24.178
5	2.422	4.049	−10.524	19.614
5.5	1.203	2.865	−6.762	6.896
6	1.331	2.140	−2.807	5.696
…				
10^{22}	**2.080**	**0**	**4.3266**	**0**
At x=0.5,				
E_{CPE} =1.6648	**3.446**	**0**	**11.875**	**0**
2	3.697	0.213	13.624	1.573
2.5	4.293	0.264	18.358	2.267
3	4.409	1.464	17.295	12.912
3.5	3.735	1.754	10.876	13.100
4	3.872	1.650	12.268	12.782
4.5	4.207	2.616	10.855	22.007
5	2.600	3.718	−7.063	19.338
5.5	1.459	2.660	−4.948	7.763
6	1.561	2.003	−1.576	6.256

10^{22}	**2.179**	**0**	**4.7484**	**0**
At x=1,				
E_{CPE} =1.8099	**3.450**	**0**	**11.905**	**0**
2	3.582	0.182	12.801	1.301
2.5	4.103	0.180	16.804	1.480
3	4.296	1.163	17.102	9.996
3.5	3.779	1.487	12.067	11.241
4	3.910	1.452	13.179	11.353
4.5	4.221	2.355	12.271	19.880
5	2.763	3.402	−3.937	18.800
5.5	1.698	2.463	−3.183	8.363
6	1.777	1.872	−0.345	6.652
…				
10^{22}	**2.274**	**0**	**5.170**	**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 $\kappa \to 0$ and $\varepsilon_2 \to 0$ as $E \to \infty$.

E in eV	n	κ	ε_1	ε_2
At x=0,				
E_{CPE} =1.5037	**4.173**	**0**	**17.414**	**0**
1.6	4.236	0.059	17.939	0.502
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	15.110	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
…				
10^{22}	**2.8057**	**0**	**7.8719**	**0**

At x=0.5,				
E_{CPE} =1.6512	**4.2147**	**0**	**17.763**	**0**
2	4.478	0.214	20.005	1.920
2.5	5.081	0.273	25.738	2.771
3	5.189	1.494	24.690	15.507
3.5	4.499	1.780	17.079	16.016
4	4.637	1.670	18.715	15.486
4.5	4.974	2.641	17.769	26.272
5	3.354	3.748	−2.805	25.143
5.5	2.205	2.679	−2.316	11.816
6	2.310	2.016	1.270	9.312
…				
10^{22}	**2.9393**	**0**	**8.6393**	**0**
At x=1,				
E_{CPE} =1.7982	**4.2508**	**0**	**18.0698**	**0**
2	4.392	0.185	19.255	1.628
2.5	4.918	0.186	24.158	1.834
3	5.106	1.186	24.662	12.114
3.5	4.576	1.508	18.671	13.803
4	4.708	1.467	20.012	13.817
4.5	5.021	2.375	19.567	23.853
5	3.551	3.427	0.869	24.339
5.5	2.480	2.478	0.007	12.293
6	2.561	1.882	3.016	9.639
…				
10^{22}	**3.0670**	**0**	**9.4067**	**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 $\eta_n(\gg 1$, 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 $\mathbf{r_d} = \mathbf{r_{As}}$,					
$\eta_n \gg 1$	↗	238	345	602	847
E_{gn1} in eV	↗	1.475	1.525	1.686	1.870
n	↘	4.247	4.201	4.046	3.865
κ	↘	2.206	2.080	1.698	1.311
ε_1	↗	13.175	13.319	13.489 ↘	13.221
ε_2	↘	18.736	17.473	13.744	10.137
For $\mathbf{r_d} = \mathbf{r_{Te}}$,					
$\eta_n \gg 1$	↗	239	345	602	847
E_{gn1} in eV	↗	1.497	1.554	1.731	1.928
n	↘	4.163	4.109	3.939	3.743
κ	↘	2.149	2.008	1.600	1.200
ε_1	↗	12.708	12.853	12.957 ↘	12.571
ε_2	↘	17.892	16.500	12.602	8.983
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↗	239	345	602	847
E_{gn1} in eV	↗	1.525	1.591	1.786	1.999
n	↘	4.054	3.992	3.802	3.587
κ	↘	2.080	1.920	1.481	1.068
ε_1		12.109 ↗	12.249 ↘	12.260	11.727
ε_2	↘	16.864	15.327	11.261	7.664
			x=0.5		
For $\mathbf{r_d} = \mathbf{r_{As}}$,					
$\eta_n \gg 1$	↗	131	189	329	463
E_{gn1} in eV	↘	1.252	1.163	1.004	0.895

n	↘	4.054	3.992	3.802	3.587
κ	↘	2.080	1.920	1.481	1.068
ε_1		12.109	↗ 12.249	↘ 12.260	11.727
ε_2	↘	16.864	15.327	11.261	7.664
			x=0.5		
For $\mathbf{r_d} = \mathbf{r_{As}}$,					
$\eta_n \gg 1$	↗	131	189	329	463
E_{gn1} in eV	↘	1.252	1.163	1.004	0.895
n	↗	4.548	4.627	4.764	4.855
κ	↗	2.812	3.074	3.575	3.940
ε_1	↘	12.777	11.953	9.911	8.050
ε_2	↗	25.585	28.448	34.067	38.256
For $\mathbf{r_d} = \mathbf{r_{Te}}$,					
$\eta_n \gg 1$	↗	131	189	329	463
E_{gn1} in eV	↘	1.284	1.206	1.069	0.979
n	↗	4.452	4.522	4.641	4.718
κ	↗	2.720	2.947	3.366	3.657
ε_1	↘	12.427	11.766	10.210	8.886
ε_2	↗	24.219	26.650	31.251	34.505
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↗	131	189	329	463
E_{gn1} in eV	↘	1.325	1.259	1.150	1.084
n	↗	4.329	4.388	4.485	4.542
κ	↗	2.606	2.791	3.115	3.320
ε_1	↘	11.951	11.465	10.409	9.611
ε_2	↗	22.570	24.501	27.942	30.156
			x=1		
For $\mathbf{r_d} = \mathbf{r_{As}}$,					
$\eta_n \gg 1$	↗	94	135	236	332
E_{gn1} in eV	↘	1.040	0.834	0.412	0.075
n	↗	4.827	5.000	5.325	5.564
κ	↗	3.457	4.151	5.760	7.241
ε_1	↘	11.342	7.758	−4.816	−21.468
ε_2	↗	33.377	41.500	61.351	80.578
For $\mathbf{r_d} = \mathbf{r_{Te}}$,					
$\eta_n \gg 1$	↗	94	135	236	332
E_{gn1} in eV	↘	1.089	0.898	0.510	0.201
n	↗	4.715	4.876	5.182	5.407
κ	↗	3.303	3.929	5.362	6.665
ε_1	↘	11.319	8.344	−1.896	−15.191

ε_2	↗	31.154	38.315	55.582	72.085
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↗	94	135	236	332
E_{gn1} in eV	↘	1.149	0.978	0.632	0.359
n	↗	4.572	4.719	4.999	5.204
κ	↗	3.117	3.661	4.888	5.983
ε_1	↘	11.191	8.871	1.099	−8.714
ε_2	↗	28.504	34.555	48.867	62.282
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 $\eta_p(\gg 1$, 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 $\mathbf{r_a} = \mathbf{r_{Ga}}$,					
$\eta_p \gg 1$	↗	**227**	335	595	**840**
E_{gp1} in eV	↗	1.869	2.043	2.466	2.869
n	↘	3.866	3.690	3.234	2.772
κ	↘	1.313	0.992	0.399	0.081
ε_1	↘	13.223	12.623	10.303	7.676
ε_2	↘	10.156	7.320	2.581	0.450
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↗	223	332	592	838
E_{gp1} in eV	↗	1.869	2.045	2.472	2.876
n	↘	3.775	3.596	3.138	2.672
κ	↘	1.312	0.988	0.393	0.077
ε_1	↘	12.529	11.953	9.692	7.135
ε_2	↘	9.909	7.106	2.468	0.415

For $r_a = r_{Cd}$,

$\eta_p \gg 1$	↗	221	330	592	837
E_{gp1} in eV	↗	1.869	2.046	2.474	2.880
n	↘	3.735	3.555	3.095	2.628
κ	↘	1.313	0.987	0.391	0.076
ε_1	↘	12.230	11.664	9.430	6.904
ε_2	↘	9.808	7.016	2.420	0.400

x=0.5

For $r_a = r_{Ga}$,

$\eta_p \gg 1$	↗	125	184	326	460
E_{gp1} in eV	↗	1.833	1.921	2.138	2.346
n	↘	4.000	3.911	3.687	3.465
κ	↘	1.385	1.212	0.836	0.540
ε_1	↘	14.083	13.831	12.901	11.712
ε_2	↘	11.077	9.482	6.165	3.743

For $r_a = r_{In}$,

$\eta_p \gg 1$	↗	124	183	325	459.6
E_{gp1} in eV	↗	1.837	1.926	2.146	2.356
n	↘	3.901	3.811	3.585	3.359
κ	↘	1.377	1.202	0.824	0.528
ε_1	↘	13.323	13.081	12.172	11.006
ε_2	↘	10.743	9.165	5.908	3.550

For $r_a = r_{Cd}$,

$\eta_p \gg 1$	↗	123.8	182.9	325.2	459.6
E_{gp1} in eV	↗	1.837	1.926	2.146	2.356
n	↘	3.901	3.811	3.585	3.359
κ	↘	1.377	1.202	0.824	0.528
ε_1	↘	13.323	13.081	12.172	11.006
ε_2	↘	10.743	9.165	5.908	3.550

x=1

For $r_a = r_{Ga}$,

$\eta_p \gg 1$	↗	90.6	132.7	234.2	330.3
E_{gp1} in eV	↗	1.912	1.970	2.114	2.254
n	↘	4.014	3.956	3.806	3.658
κ	↘	1.229	1.121	0.874	0.663
ε_1	↘	14.604	14.390	13.725	12.940
ε_2	↘	9.867	8.871	6.651	4.848

For $r_a = r_{In}$,

$\eta_p \gg 1$	↗	89.6	131.9	233.6	329.8
E_{gp1} in eV	↗	1.917	1.976	2.123	2.265
n	↘	3.910	3.850	3.698	3.548
κ	↘	1.220	1.110	0.860	0.648
ε_1	↘	13.803	13.593	12.939	12.165
ε_2	↘	9.541	8.551	6.364	4.600

For $r_a = r_{Cd}$,

$\eta_p \gg 1$	↗	89.1	131.4	233.3	329.5
E_{gp1} in eV	↗	1.919	1.979	2.126	2.269

n	↘	3.865	3.804	3.651	3.499
κ	↘	1.216	1.106	0.854	0.642
ε_1	↘	13.457	13.249	12.600	11.831
ε_2	↘	9.398	8.412	6.238	4.493
N (10^{18} cm^{-3})	↗	15	26	60	100

Table 5n: In the X(x)-system, at E=3.2 eV and $N = 10^{20} cm^{-3}$, for given r_d and x, and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of $\eta_n (\gg 1$, degenerate case$)$, E_{gn1}, n, κ, ε_1 and ε_2, obtained as functions of T, being represented by the arrows: ↗ and ↘, noting that both η_n and E_{gn1} decrease with increasing T.

T in K	↗	20	50	100	300	
			x=0			
For $r_d = r_{As}$,						
$\eta_n \gg 1$	↘	847	339	169	56	
E_{gn1} in eV	↘	1.870	1.866	1.853	1.774	
n	↗	3.865	3.870		3.882	3.961
κ	↗	1.311	1.320	1.345	1.507	
ε_1	↗	13.221	13.232	13.263	13.415	
ε_2	↗	10.132	10.215	10.441	11.940	
For $r_d = r_{Te}$,						
$\eta_n \gg 1$	↘	847	339	169	56	
E_{gn1} in eV	↘	1.928	1.923	1.911	1.832	
n	↗	3.743	3.747	3.760	3.839	
κ	↗	1.200	1.208	1.232	1.388	
ε_1	↗	12.571	12.584	12.621	12.816	
ε_2	↗	8.983	9.055	9.264	10.656	
For $r_d = r_{Sn}$,						
$\eta_n \gg 1$	↘	847	339	169	56	
E_{gn1} in eV	↘	1.999	1.995	1.983	1.904	
n	↗	3.587	3.592	3.604	3.685	
κ	↗	1.068	1.076	1.098	1.246	
ε_1	↗	11.727	11.742	11.785	12.026	
ε_2	↗	7.664	7.729	7.919	9.181	

x=0.5

For $\mathbf{r_d} = \mathbf{r_{As}}$,					
$\eta_n \gg 1$	↘	463	185	93	31
E_{gn1} in eV	↘	0.895	0.887	0.869	0.765
n	↗	4.855	4.861	4.876	4.960
κ	↗	3.940	3.964	4.028	4.395
ε_1	↘	8.050	7.914	7.551	5.292
ε_2	↗	38.256	38.542	39.287	43.600
For $\mathbf{r_d} = \mathbf{r_{Te}}$,					
$\eta_n \gg 1$	↘	463	185	93	31
E_{gn1} in eV	↘	0.979	0.972	0.953	0.849
n	↗	4.718	4.724	4.739	4.825
κ	↗	3.657	3.680	3.742	4.096
ε_1	↘	8.886	8.769	8.459	6.508
ε_2	↗	34.505	34.773	35.472	39.525
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↘	463	185	93	31
E_{gn1} in eV	↘	1.084	1.077	1.058	0.954
n	↗	4.542	4.548	4.564	4.652
κ	↗	3.320	3.342	3.401	3.738
ε_1	↘	9.611	9.517	9.265	7.666
ε_2	↗	30.156	30.403	31.046	34.781

x=1

For $\mathbf{r_d} = \mathbf{r_{As}}$,					
$\eta_n \gg 1$	↘	332	133	66	22
E_{gn1} in eV	↘	0.075	0.065	0.040	−0.088
n	↗	5.564	5.571	5.587	5.672
κ	↗	7.241	7.287	7.402	8.016
ε_1	↘	−21.467	−22.067	−23.576	−32.082
ε_2	↗	80.578	81.193	82.723	90.929
For $\mathbf{r_d} = \mathbf{r_{Te}}$,					
$\eta_n \gg 1$	↘	332	133	66	22
E_{gn1} in eV	↘	0.201	0.191	0.167	0.038
n	↗	5.407	5.414	5.431	5.519
κ	↗	6.665	6.710	6.821	7.410
ε_1	↘	−15.191	−15.711	−17.023	−24.451
ε_2	↗	72.085	72.660	74.093	81.787
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↘	332	133	66	22
E_{gn1} in eV	↘	0.359	0.349	0.324	0.196
n	↗	5.204	5.212	5.230	5.321
κ	↗	5.983	6.026	6.130	6.690
ε_1	↘	−8.714	−9.145	−10.234	−16.443
ε_2	↗	62.282	62.809	64.122	71.189
T in K	↗	20	50	100	300

Table 5p: In the X(x)-system, at E=3.2 eV and $N = 10^{20} cm^{-3}$, for given r_a and x, and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of $\eta_p (\gg 1$, 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 $\mathbf{r_a} = \mathbf{r_{Ga}}$,						
$\eta_p \gg 1$	↘	840	336	168	56	
E_{gp1} in eV	↘	2.869	2.865	2.852	2.773	
n	↗	2.772	2.777		2.792	2.885
κ	↗	0.081	0.083	0.090	0.135	
ε_1	↗	7.676	7.704	7.785	8.303	
ε_2	↗	0.450	0.463	0.501	0.779	
For $\mathbf{r_a} = \mathbf{r_{In}}$,						
$\eta_p \gg 1$	↘	838	335	168	56	
E_{gp1} in eV	↘	2.876	2.872	2.860	2.780	
n	↗	2.672	2.677		2.692	2.785
κ	↗	0.077	0.080	0.086	0.130	
ε_1	↗	7.135	7.162	7.241	7.741	
ε_2	↗	0.415	0.427	0.462	0.726	
For $\mathbf{r_a} = \mathbf{r_{Cd}}$,						
$\eta_p \gg 1$	↘	837	335	167	56	
E_{gp1} in eV	↘	2.880	2.875	2.863	2.784	
n	↗	2.628	2.634		2.648	2.742
κ	↗	0.076	0.078	0.084	0.128	
ε_1	↗	6.904	6.931	7.008	7.500	
ε_2	↗	0.400	0.412	0.446	0.704	
			x=0.5			
For $\mathbf{r_a} = \mathbf{r_{Ga}}$,						
$\eta_p \gg 1$	↘	460	184	92	31	
E_{gp1} in eV	↘	2.346	2.339	2.320	2.217	

n	↗	3.465	3.472	3.493	3.604
κ	↗	0.540	0.549	0.573	0.716
ε_1	↗	11.712	11.756	11.870	12.477
ε_2	↗	3.743	3.815	4.005	5.165
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↘	460	184	92	30.6
E_{gp1} in eV	↘	2.356	2.349	2.330	2.226
n	↗	3.359	3.367	3.387	3.499
κ	↗	0.528	0.537	0.561	0.703
ε_1	↗	11.006	11.049	11.160	11.751
ε_2	↗	3.550	3.619	3.801	4.919
For $\mathbf{r_a} = \mathbf{r_{Cd}}$,					
$\eta_p \gg 1$	↘	459	184	92	30
E_{gp1} in eV	↘	2.360	2.353	2.334	2.230
n	↗	3.313	3.321	3.341	3.453
κ	↗	0.523	0.532	0.556	0.697
ε_1	↗	10.702	10.745	10.854	11.437
ε_2	↗	3.466	3.534	3.713	4.812
			x=1		
For $\mathbf{r_a} = \mathbf{r_{Ga}}$,					
$\eta_p \gg 1$	↘	330	132	66	22
E_{gp1} in eV	↘	2.254	2.244	2.220	2.091
n	↗	3.658	3.668	3.695	3.830
κ	↗	0.663	0.677	0.712	0.911
ε_1	↗	12.940	13.000	13.145	13.842
ε_2	↗	4.848	4.966	5.263	6.978
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↘	330	132	66	22
E_{gp1} in eV	↘	2.265	2.255	2.230	2.102
n	↗	3.548	3.558	3.585	3.720
κ	↗	0.648	0.662	0.697	0.894
ε_1	↗	12.165	12.223	12.365	13.043
ε_2	↗	4.600	4.713	5.000	6.653
For $\mathbf{r_a} = \mathbf{r_{Cd}}$,					
$\eta_p \gg 1$	↘	329	132	66	22
E_{gp1} in eV	↘	2.269	2.259	2.235	2.106
n	↗	3.499	3.510	3.536	3.672
κ	↗	0.642	0.656	0.691	0.887
ε_1	↗	11.831	11.889	12.028	12.698
ε_2	↗	4.493	4.604	4.886	6.512
T in K	↗	20	50	100	300