wjert, 2024, Vol. 10 Issue 12, 400-421. *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 InP(1-x) Sb(x)-CRYSTALLINE ALLOY, DUE TO THE NEW STATIC DIELECTRIC CONSTANT-LAW AND THE GENERALIZED MOTT CRITERIUM IN THE METAL-INSULATOR TRANSITION (21)

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Article Received on 21/10/2024 **Article Revised on 11/11/2024** **Article Accepted on 01/12/2024**

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ABTRACT

In the n(p)-type $\mathbf{X(x) \equiv InP_{1-x}Sb_x}$- 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 $\mathbf{2.91 \times 10^{-7}}$, as that given in Table 4 of Ref.[1], according to a definition of the effective density of electrons (holes) given in parabolic conduction (valence) bands by: $N^*(N, r_{d(a)}, x) \equiv N - N_{CDn(NDp)}(r_{d(a)}, x)$, as defined in Eq. (9d). In summary, due to the new $\varepsilon(r_{d(a)}, x)$-law and to the effective density of electrons (holes) given in parabolic conduction (valence) bands $N^*(N, r_{d(a)}, x)$, for a given x, and with an increasing $r_{d(a)}$, the numerical results of all the optical coefficients, obtained in appropriated physical conditions (E, N, T),

and calculated by using Equations (15, 16, 20, 21), are reported in Tables 1, 2, 3n, 3p, 4n, 4p, 5n, and 5p in Appendix 1.

KEYWORS: $InP_{1-x}Sb_x$- 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 $\mathbf{X(x) \equiv InP_{1-x}Sb_x}$- 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: $\mathbf{r_{do(ao)}=r_{P(In)}}$**=0.110 nm (0.144 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:

$$m_{c(v)}(x)/m_o = 0.1\ (0.4) \times x + 0.077(0.5) \times (1 - x) \tag{1}$$

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

$$\varepsilon_o(x) = 16.8 \times x + 12.5 \times (1 - x). \tag{2}$$

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

$$E_{go}(x) = 0.23 \times x + 1.424 \times (1 - x). \tag{3}$$

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

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

and then, the isothermal bulk modulus, by:

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

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 $V = (4\pi/3)\times(r_{d(a)})^3$, $V_{do(ao)} = (4\pi/3)\times(r_{do(ao)})^3$, 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:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

being equal to, in particular, at N=$N_{CDn(CDp)}(r_{d(a)},x)$: $r_{sn(sp)}\left(N_{CDn(CDp)}(r_{d(a)},x), r_{d(a)},x\right)$= **2.4813963**, for any $(r_{d(a)},x)$-values. So, from Eq. (9b), one also has :

$$N_{CDn(CDp)}(r_{d(a)},x)^{1/3} \times a_{Bn(Bp)}(r_{d(a)},x) = \left(\frac{3}{4\pi}\right)^{\frac{1}{3}} \times \frac{1}{2.4813963} = \mathbf{0.25} = (\mathbf{WS})_{\mathbf{n(p)}} = \mathbf{M}_{\mathbf{n(p)}}. \quad (9c)$$

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

Furthermore, by using $\mathbf{M}_{\mathbf{n(p)}} = \mathbf{0.25}$, according to the empirical Heisenberg parameter $\boldsymbol{\mathcal{H}}_{\mathbf{n(p)}} = \mathbf{0.47137}$, as those given in Equations (8, 15) of the Ref.[1], we have also showed that $N_{CDn(CDp)}$ is just the density of electrons (holes) localized in the exponential conduction (valence)-band tail, with a precision of the order of $\mathbf{2.91} \times \mathbf{10^{-7}}$. Therefore, the density of electrons (holes) given in parabolic conduction (valence) bands can be defined, as that given in compensated materials, by:

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

C. Effect of temperature T, with given x and $\mathbf{r_{d(a)}}$

Here, the intrinsic band gap $E_{gni(gpi)}(r_{d(a)},x,T)$ at any T is given by:

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

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:

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

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 $\mathbf{r_{d(a)}}$

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) $\frac{E_{Fn}(u \ll 1)}{k_B T}\left(\frac{-E_{Fp}(u \ll 1)}{k_B T}\right) \ll -1$, to the LD [a(d)- X(x)- alloy] BR-case, or to the non-degenerate case, Eq. (12) is reduced to the function G(u), noting that the notations: **HD(LD)** and **ER(BR)** denote the heavily doped (lightly doped)-cases and emitter (base)-regions, respectively.

Now, in Eq. (9b), in which one replaces $m_{c(v)}(x)$ by $m_r(x)$, the effective Wigner-Seitz radius becomes as:

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

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

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

Then, taking into account various spin-polarized chemical potential-energy contributions such as: exchange energy of an effective electron (hole) gas, majority-carrier correlation energy of an effective electron (hole) gas, minority hole (electron) correlation energy, majority electron (hole)-ionized d(a) interaction screened Coulomb potential energy, and finally minority hole (electron)-ionized d(a) interaction screened Coulomb potential energy, the band gap narrowings are given in the following.

In the n-type HD X(x)- alloy, the BGN is found to be given by:

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

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

$$\Delta E_{gn}(N, r_d, x) = \Delta E_{gno}(N, r_d, x) \times \{1.1 \times x + 1.3 \times (1 - x)\}, \quad (14n)$$

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:

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

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

$$\Delta E_{gp}(N, r_a, x) = \Delta E_{gpo}(N, r_a, x) \times \{9 \times x + 22 \times (1 - x)\}, \quad (14p)$$

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, $\Delta E_{gn(gp)}(N, r_{d(a)}, x) = 0$.

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]

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

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

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

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

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

Then, one has:

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

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

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

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

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

$$= F(E) \times \left(E^* \equiv E - E_{gn1(gp1)}\right)^2$$, for $E \geq 2.3$ 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 $n(E \to \infty, r_{d(a)}, x) \to n_\infty(r_{d(a)}, x) = \sqrt{\varepsilon(r_{d(a)}, x)} \times \frac{\omega_T}{\omega_L}$, $\omega_T = 5.1 \times 10^{13}\ s^{-1}$ [5] and $\omega_L = 8.9755 \times 10^{13}\ s^{-1}$.

Here, the other parameters are determined by: $X_i\left(E_{gn1(gp1)}\right) = \frac{A_i}{Q_i} \times \left[-\frac{B_i^2}{2} + E_{gn1(gp1)} B_i - E_{gn1(gp1)}^2 + C_i\right]$, $Y_i\left(E_{gn1(gp1)}\right) = \frac{A_i}{Q_i} \times \left[\frac{B_i \times (E_{gn1(gp1)}^2 + C_i)}{2} - 2E_{gn1(gp1)} C_i\right]$, $Q_i = \frac{\sqrt{4C_i - B_i^2}}{2}$, where, for i=(1, 2, 3, and 4), $A_i = 1.154 \times A_{i(FB)} = 4.7314 \times 10^{-4}, 0.2314, 0.1118$ and 0.0116, $B_i \equiv B_{i(FB)} = 5.871, 6.154, 9.679$ and 13.232, and $C_i \equiv C_{i(FB)} = 8.619, 9.784, 23.803$, and 44.119.

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

NUMERICAL RESULTS

Now, some numerical results of those optical functions are investigated in the n(p)-type $\mathbf{X(x) \equiv InP_{1-x}Sb_x}$- 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 $\propto_{MIT}(r_{d(a)}, x) = 0$, 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, in which T=0K and $N = N_{CDn(CDp)}$.

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

In the P(Ga)-X(x)-system, at T=0K and $N = N_{CDn(CDp)}(r_{P(Ga)}, x)$, our numerical results of n, κ, ε_1 and ε_2 are obtained from Equations (21, 20, 16), respectively, and expressed as functions of E [$\geq E_{CPE}(r_{P(Ga)}, x)$] and for given x, as those reported in Tables 3n and 3p in Appendix 1.

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

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

E. Variations of various optical coefficients as functions of T

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

CONCLUDING REMARKS

In the n(p)-type $\mathbf{X(x) \equiv InP_{1-x}Sb_x}$- 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 $\mathbf{2.91 \times 10^{-7}}$, as that given in Table 4 of Ref.[1], according to a definition of the effective density of electrons (holes) given in parabolic conduction (valence) bands by: $N^*(N, r_{d(a)}, x) \equiv N - N_{CDn(NDp)}(r_{d(a)}, x)$, as defined in Eq. (9d).

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

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APPENDIX 1

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

Donor		P	As	Sb	Sn
r_d (nm) [4]	↗	0.110	0.118	0.136	0.140
At **x=0**,					
E_{CPE} in meV	↗	1424	1424.3	1427.8	1429
n_{MIT}	↘	3.426	3.402	3.210	3.156
$\varepsilon_{1(MIT)}$	↘	11.74	11.57	10.31	9.96
R_{MIT}	↘	0.300	0.298	0.276	0.269
At **x=0.5**,					
E_{CPE} in meV	↗	827	827.3	830.2	831.3
n_{MIT}	↘	3.964	3.938	3.731	3.672
$\varepsilon_{1(MIT)}$	↘	15.71	15.50	13.92	13.49
R_{MIT}	↘	0.356	0.354	0.333	0.327
At **x=1**,					
E_{CPE} in meV	↗	230	230.2	232.7	233.7
n_{MIT}	↘	4.490	4.462	4.241	4.178
$\varepsilon_{1(MIT)}$	↘	20.16	19.91	17.99	17.46
R_{MIT}	↘	0.404	0.402	0.382	0.377

Acceptor		Ga	Mg	In	Cd
r_a (nm)	↗	0.126	0.140	0.144	0.148
At **x=0**,					
E_{CPE} in meV	↗	1418.2	1423.7	1424	1424.3
n_{MIT}	↘	3.502	3.429	3.426	3.422
$\varepsilon_{1(MIT)}$	↘	12.26	11.76	11.74	11.71
R_{MIT}	↘	0.309	0.301	0.3002	0.300
At **x=0.5**,					
E_{CPE} in meV	↗	823.2	826.8	827	827.2
n_{MIT}	↘	4.045	3.968	3.964	3.960
$\varepsilon_{1(MIT)}$	↘	16.36	15.74	15.71	15.68
R_{MIT}	↘	0.364	0.357	0.3565	0.3561
At **x=1**,					
E_{CPE} in meV	↗	227.4	229.87	230	230.1
n_{MIT}	↘	4.576	4.494	4.490	4.486
$\varepsilon_{1(MIT)}$	↘	20.94	20.20	20.16	20.12
R_{MIT}	↘	0.411	0.4045	0.4041	0.4038

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

Donor		P	As	Sb	Sn
At **x=0**,					
n_∞	↘	2.009	1.985	1.796	1.742
$\varepsilon_{1,\infty}$	↘	4.036	3.940	3.225	3.035

$\sigma_{o,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	9.167	9.057	8.194	7.950
$\propto_\infty$ in $(10^9 \times cm^{-1}) = 2.1602$					
R_∞	↘	0.112	0.109	0.081	0.073
At **x=0.5**,					
n_∞	↘	2.175	2.149	1.944	1.886
$\varepsilon_{1,\infty}$	↘	4.730	4.617	3.779	3.557
$\sigma_{o,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	9.924	9.805	8.871	8.606
$\propto_\infty$ in $(10^9 \times cm^{-1}) = 2.1602$					
R_∞	↘	0.137	0.133	0.103	0.094
At **x=1**,					
n_∞	↘	2.329	2.301	2.082	2.020
$\varepsilon_{1,\infty}$	↘	5.424	5.295	4.334	4.079
$\sigma_{o,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	10.627	10.500	9.499	9.216
$\propto_\infty$ in $(10^9 \times cm^{-1}) = 2.1602$					
R_∞	↘	0.159	0.155	0.123	0.114

Acceptor		Ga	Mg	In	Cd
At **x=0**,					
n_∞	↘	2.081	2.012	2.009	2.005
$\varepsilon_{1,\infty}$	↘	4.332	4.050	4.036	4.022
$\sigma_{o,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	9.50	9.18	9.167	9.151
$\propto_\infty$ in $(10^9 \times cm^{-1}) = 2.1602$					
R_∞	↘	0.123	0.113	0.112	0.1119
At **x=0.5**,					
n_∞	↘	2.253	2.178	2.175	2.171
$\varepsilon_{1,\infty}$	↘	5.077	4.746	4.730	4.713
$\sigma_{o,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	10.28	9.941	9.924	9.907
$\propto_\infty$ in $(10^9 \times cm^{-1}) = 2.1602$					
R_∞	↘	0.148	0.137	0.137	0.1364
At **x=1**,					
n_∞	↘	2.413	2.333	2.329	2.325
$\varepsilon_{1,\infty}$	↘	5.823	5.443	5.424	5.405
$\sigma_{o,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	11.01	10.64	10.63	10.61
$\propto_\infty$ in $(10^9 \times cm^{-1}) = 2.1602$					
R_∞	↘	0.171	0.160	0.159	0.15878

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

E in eV	n	κ	ε_1	ε_2
At x=0,				
$\mathbf{E_{CPE} = 1.424}$	**3.4259**	**0**	**11.7371**	**0**
2	3.910	0.221	15.239	1.725
2.5	4.638	0.438	21.320	4.066
3	4.590	2.040	16.910	18.731
3.5	3.626	2.244	8.113	16.275
4	3.779	2.008	10.245	15.180
4.5	4.158	3.079	7.814	25.608

5	2.293	4.275	−13.015	19.603
5.5	1.022	3.005	−7.985	6.142
6	1.168	2.232	−3.619	5.213
…				
10^{22}	**2.0089**	**0**	**4.0358**	**0**
At x=0.5,				
E_{CPE} =0.827	**3.9639**	**0**	**15.7123**	**0**
2	5.214	0.139	27.162	1.453
2.5	6.316	1.060	38.769	13.385
3	5.665	3.879	17.046	43.945
3.5	3.817	3.720	0.726	28.400
4	4.041	3.047	7.043	24.630
4.5	4.564	4.390	1.560	40.075
5	1.987	5.821	−29.937	23.131
5.5	0.378	3.950	−15.457	2.984
6	0.657	2.853	−7.706	3.750
…				
10^{22}	**2.1748**	**0**	**4.7300**	**0**
At x=1,				
E_{CPE} =0.23	**4.4900**	**0**	**20.1602**	**0**
2	6.774	0.025	45.890	0.340
2.5	8.316	1.951	65.344	32.444
3	6.780	6.303	6.241	85.463
3.5	3.815	5.568	−16.448	42.481
4	4.157	4.302	−1.228	35.767
4.5	4.869	5.933	−11.495	57.777
5	1.482	7.606	−55.652	22.537
5.5	−0.490	5.023	−24.993	−4.927
6	−0.039	3.549	−12.594	−0.275
…				
10^{22}	**2.3290**	**0**	**5.4241**	**0**
E in eV	n	κ	ε_1	ε_2

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

E in eV	n	κ	ε_1	ε_2
At x=0,				
E_{CPE} =1.4182	**3.5020**	**0**	**12.2643**	**0**
2	3.992	0.220	15.889	1.759
2.5	4.724	0.443	22.117	4.183
3	4.671	2.055	17.599	19.201
3.5	3.700	2.257	8.596	16.698
4	3.853	2.017	10.774	15.547
4.5	4.234	3.090	8.374	26.169
5	2.362	4.288	−12.812	20.256
5.5	1.088	3.013	−7.897	6.556
6	1.234	2.238	−3.484	5.525
…				
10^{22}	**2.0814**	**0**	**4.3324**	**0**
At x=0.5,				
E_{CPE} =0.8232	**4.0447**	**0**	**16.3598**	**0**
2	5.300	0.139	28.072	1.469
2.5	6.405	1.064	39.893	13.635
3	5.749	3.892	17.905	44.754

3.5	3.895	3.731	1.250	29.063
4	4.120	3.055	7.641	25.169
4.5	4.644	4.399	2.215	40.859
5	2.062	5.831	−29.756	24.046
5.5	0.450	3.956	−15.447	3.564
6	0.731	2.857	−7.627	4.176
…				
10^{22}	**2.2533**	**0**	**5.0776**	**0**
At x=1,				
E_{CPE} =0.2274	**4.5756**	**0**	**20.9366**	**0**
2	6.865	0.025	7.126	0.339
2.5	8.408	1.955	66.876	32.879
3	6.868	6.314	7.300	86.735
3.5	3.898	5.576	−15.905	43.473
4	4.240	4.308	−0.576	36.536
4.5	4.953	5.940	−10.749	58.850
5	1.562	7.614	−55.530	23.792
5.5	−0.411	5.028	−25.113	−4.135
6	0.041	3.552	−12.616	0.293
…				
10^{22}	**2.4130**	**0**	**5.8228**	**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 $\mathbf{r_d} = \mathbf{r_P}$,					
$\eta_n \gg 1$	↗	192.6	278	486	683
E_{gn1} in eV	↗	1.298	1.316	1.398	1.506
n	↘	4.359	4.343	4.269	4.169
κ	↘	2.680	2.632	2.408	2.128
ε_1	↗	11.816	11.937	12.424	12.849
ε_2	↘	23.367	22.865	20.561	17.743
For $\mathbf{r_d} = \mathbf{r_{Sb}}$,					
$\eta_n \gg 1$	↗	192.4	277.8	485.6	682.7
E_{gn1} in eV	↗	1.368	1.407	1.536	1.685
n	↘	4.083	4.047	3.926	3.784
κ	↘	2.489	2.384	2.051	1.700
ε_1	↗	10.477	10.698	11.209	11.428
ε_2	↘	20.324	19.295	16.110	12.870
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↗	192.3	277.79	485.5	682.67
E_{gn1} in eV	↗	1.384	1.428	1.569	1.727
n	↘	4.015	3.974	3.842	3.690
κ	↘	2.445	2.327	1.972	1.608
ε_1	↗	10.139	10.376	10.874	11.030
ε_2	↘	19.633	18.499	15.158	11.867
x=0.5					

For $\mathbf{r_d} = \mathbf{r_P}$,					
$\eta_n \gg 1$	↗	173.8	250.8	438.2	616.1
E_{gn1} in eV	↗	0.698	0.708	0.770	0.858
n	↘	5.032	5.024	4.974	4.903
κ	↘	4.640	4.603	4.376	4.067
ε_1	↗	3.785	4.051	5.592	7.503
ε_2	↘	46.697	46.248	43.535	39.882
For $\mathbf{r_d} = \mathbf{r_{Sb}}$,					
$\eta_n \gg 1$	↗	173.6	250.7	438.1	615.97
E_{gn1} in eV	↗	0.764	0.795	0.903	1.029
n	↘	4.748	4.723	4.635	4.529
κ	↘	4.399	4.287	3.912	3.493
ε_1	↗	3.198	3.930	6.184	8.313
ε_2	↘	41.774	40.501	36.266	31.644
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↗	173.5	250.6	438.0	615.94
E_{gn1} in eV	↗	0.779	0.815	0.934	1.069
n	↘	4.678	4.649	4.552	4.437
κ	↘	4.343	4.215	3.807	3.366
ε_1	↗	3.021	3.845	6.222	8.361
ε_2	↘	40.635	39.194	34.663	29.873
			x=1		
For $\mathbf{r_d} = \mathbf{r_P}$,					
$\eta_n \gg 1$	↗	160.6	231.9	405.1	569.5
E_{gn1} in eV	↗	0.110	0.119	0.174	0.253
n	↘	5.618	5.612	5.574	5.519
κ	↘	7.076	7.038	6.787	6.438
ε_1	↗	−18.508	−18.029	−14.991	−10.985
ε_2	↘	79.511	78.997	75.667	71.061
For $\mathbf{r_d} = \mathbf{r_{Sb}}$,					
$\eta_n \gg 1$	↗	160.5	231.8	405.0	569.4
E_{gn1} in eV	↗	0.172	0.201	0.299	0.414
n	↘	5.328	5.309	5.239	5.155
κ	↘	6.794	6.669	6.239	5.752
ε_1	↗	−17.775	−16.291	−11.481	−6.514
ε_2	↘	72.407	70.807	65.380	59.312
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↗	160.4	231.7	404.97	569.4
E_{gn1} in eV	↗	0.187	0.220	0.328	0.452
n	↘	5.256	5.233	5.156	5.065
κ	↘	6.729	6.584	6.115	5.599
ε_1	↗	−17.659	−15.965	−10.809	−5.686
ε_2	↘	70.743	68.915	63.065	56.719
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 $\mathbf{r_a} = \mathbf{r_{Ga}}$,					
$\eta_p \gg 1$	↗	142.9	238	456	658
E_{gp1} in eV	↗	1.290	1.310	1.414	1.544
n	↘	4.439	4.421	4.327	4.205
κ	↘	2.704	2.647	2.366	2.031
ε_1	↗	12.392	12.537	13.124	13.552
ε_2	↘	24.008	23.401	20.471	17.084
For $\mathbf{r_a} = \mathbf{r_{Mg}}$,					
$\eta_p \gg 1$	↗	130.5	228.5	449	652
E_{gp1} in eV	↗	1.307	1.332	1.447	1.589
n	↘	4.355	4.332	4.226	4.093
κ	↘	2.657	2.587	2.277	1.923
ε_1	↗	11.906	12.075	12.679	13.056
ε_2	↘	23.138	22.417	19.244	15.738
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↗	129.8	227.9	448.8	652
E_{gp1} in eV	↗	1.308	1.333	1.449	1.592
n	↘	4.351	4.330	4.221	4.087
κ	↘	2.654	2.584	2.272	1.917
ε_1	↗	11.882	12.052	12.656	13.030
ε_2	↘	23.097	22.370	19.185	15.674
x=0.5					
For $\mathbf{r_a} = \mathbf{r_{Ga}}$,					
$\eta_p \gg 1$	↗	154.4	234.9	426	606
E_{gp1} in eV	↗	0.673	0.681	0.746	0.840
n	↘	5.130	5.123	5.072	4.996
κ	↘	4.732	4.702	4.462	4.130
ε_1	↗	3.919	4.136	5.809	7.911
ε_2	↘	48.549	48.183	45.265	41.268
For $\mathbf{r_a} = \mathbf{r_{Mg}}$,					
$\eta_p \gg 1$	↗	149.8	231.2	423	604
E_{gp1} in eV	↗	0.692	0.706	0.785	0.889
n	↘	5.039	5.029	4.966	4.881
κ	↘	4.660	4.609	4.325	3.958
ε_1	↗	3.684	4.044	5.961	8.157
ε_2	↘	46.967	46.357	42.960	38.645
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↗	149.5	231.0	423	603.6
E_{gp1} in eV	↗	0.694	0.708	0.786	0.892
n	↘	5.035	5.024	4.961	4.875
κ	↘	4.656	4.605	4.318	3.950
ε_1	↗	3.671	4.039	5.967	8.166

ε_2	↘	46.889	46.268	42.847	38.519
		x=1			
For $\mathbf{r_a = r_{Ga}}$,					
$\eta_p \gg 1$	↗	152.5	225.2	400	565
E_{gp1} in eV	↗	0.138	0.159	0.245	0.351
n	↘	5.684	5.669	5.609	5.533
κ	↘	6.952	6.856	6.475	6.018
ε_1	↗	−16.032	−14.870	−10.461	−5.598
ε_2	↘	79.031	77.737	72.635	66.591
For $\mathbf{r_a = r_{Mg}}$,					
$\eta_p \gg 1$	↗	150.6	223.6	398.9	564.3
E_{gp1} in eV	↗	0.154	0.181	0.278	0.393
n	↘	5.592	5.574	5.506	5.422
κ	↘	6.877	6.758	6.331	5.839
ε_1	↗	−16.022	−14.609	−9.769	−4.696
ε_2	↘	76.916	75.343	69.711	63.314
For $\mathbf{r_a = r_{In}}$,					
$\eta_p \gg 1$	↗	150.5	223.5	398.8	564.2
E_{gp1} in eV	↗	0.155	0.182	0.279	0.396
n	↘	5.588	5.569	5.500	5.416
κ	↘	6.873	6.754	6.324	5.830
ε_1	↗	−16.022	−14.597	−9.737	−4.654
ε_2	↘	76.812	75.225	69.569	63.154
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 $\eta_n (\gg 1, \text{degenerate case})$, E_{gn1}, n, κ, ε_1 and ε_2, obtained as functions of T, being represented by the arrows: ↗ and ↘, noting that both η_n and E_{gn1} decrease with increasing T.

T in K	↗	20	50	100	300
		x=0			
For $\mathbf{r_d = r_P}$,					
$\eta_n \gg 1$	↘	682.8	273	136	45
E_{gn1} in eV	↘	1.506	1.496	1.471	1.343
n	↗	4.169	4.178	4.201	4.318
κ	↗	2.128	2.153	2.216	2.556
ε_1	↘	12.849	12.820	12.738	12.117
ε_2	↗	17.743	17.994	18.620	22.077
For $\mathbf{r_d = r_{Sb}}$,					
$\eta_n \gg 1$	↘	682.7	273	136	45
E_{gn1} in eV	↘	1.685	1.675	1.651	1.523
n	↗	3.784	3.794	3.818	3.939
κ	↗	1.700	1.723	1.779	2.085
ε_1	↘	11.428	11.424	11.409	11.171
ε_2	↗	12.870	13.074	13.585	16.428
For $\mathbf{r_d = r_{Sn}}$,					
$\eta_n \gg 1$	↘	682.6	273	136	45

E_{gn1} in eV	↘	1.727	1.717	1.692	1.565
n	↗	3.690	3.700	3.724	3.846
κ	↗	1.608	1.630	1.685	1.982
ε_1	↘	11.030	11.031	11.028	10.864
ε_2	↗	11.867	12.060	12.546	15.251
x=0.5					
For $\mathbf{r_d} = \mathbf{r_P}$,					
$\eta_n \gg 1$	↘	616	246.4	123.2	41.05
E_{gn1} in eV	↘	0.858	0.851	0.832	0.728
n	↗	4.903	4.909	4.924	5.008
κ	↗	4.067	4.092	4.157	4.528
ε_1	↘	7.503	7.357	6.970	4.571
ε_2	↗	39.882	40.175	40.939	45.353
For $\mathbf{r_d} = \mathbf{r_{Sb}}$,					
$\eta_n \gg 1$	↘	615.97	246.4	123.2	41.04
E_{gn1} in eV	↘	1.029	1.022	1.003	0.900
n	↗	4.529	4.535	4.551	4.638
κ	↗	3.493	3.516	3.577	3.922
ε_1	↘	8.313	8.206	7.922	6.129
ε_2	↗	31.644	31.897	32.556	36.377
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↘	615.94	246.37	123.18	41.04
E_{gn1} in eV	↘	1.069	1.062	1.043	0.940
n	↗	4.437	4.444	4.459	4.547
κ	↗	3.366	3.389	3.448	3.787
ε_1	↘	8.361	8.262	7.998	6.332
ε_2	↗	29.873	30.117	30.752	34.437
		x=1			
For $\mathbf{r_d} = \mathbf{r_P}$,					
$\eta_n \gg 1$	↘	569.5	227.8	113.9	37.95
E_{gn1} in eV	↘	0.253	0.249	0.236	0.157
n	↗	5.519	5.522	5.531	5.586
κ	↗	6.438	6.457	6.512	6.864
ε_1	↘	−10.985	−11.197	−11.811	−15.916
ε_2	↗	71.061	71.312	72.032	76.695
For $\mathbf{r_d} = \mathbf{r_{Sb}}$,					
$\eta_n \gg 1$	↘	569.4	227.77	113.88	37.94
E_{gn1} in eV	↘	0.414	0.410	0.397	0.318
n	↗	5.155	5.158	5.168	5.225
κ	↗	5.752	5.770	5.822	6.156
ε_1	↘	−6.514	−6.689	−7.195	−10.596
ε_2	↗	59.312	59.535	60.177	64.338
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↘	569.4	227.76	113.87	37.94
E_{gn1} in eV	↘	0.452	0.447	0.435	0.356
n	↗	5.065	5.069	5.078	5.136
κ	↗	5.599	5.616	5.668	5.997
ε_1	↘	−5.686	−5.583	−6.336	−9.585
ε_2	↗	56.719	56.936	57.560	61.604

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 $\mathbf{r_a = r_{Ga}}$,					
$\eta_p \gg 1$	↘	658	263	131	44
E_{gp1} in eV	↘	1.544	1.535	1.510	1.382
n	↗	4.205	4.214	4.237	4.356
κ	↗	2.031	2.056	2.117	2.450
ε_1	↘	13.552	13.531	13.471	12.969
ε_2	↗	17.084	17.329	17.945	21.343
For $\mathbf{r_a = r_{Mg}}$,					
$\eta_p \gg 1$	↘	652	261	130	43.5
E_{gp1} in eV	↘	1.589	1.579	1.555	1.427
n	↗	4.093	4.102	4.126	4.245
κ	↗	1.923	1.946	2.006	2.330
ε_1	↘	13.056	13.041	12.997	12.592
ε_2	↗	15.738	15.971	16.555	19.785
For $\mathbf{r_a = r_{In}}$,					
$\eta_p \gg 1$	↘	652	260.8	130	43.4
E_{gp1} in eV	↘	1.592	1.582	1.557	1.429
n	↗	4.087	4.097	4.120	4.240
κ	↗	1.917	1.941	2.001	2.324
ε_1	↘	13.030	13.016	12.973	12.573
ε_2	↗	15.674	15.907	16.489	19.711
		x=0.5			
For $\mathbf{r_a = r_{Ga}}$,					
$\eta_p \gg 1$	↘	606	242	121	40
E_{gp1} in eV	↘	0.840	0.833	0.814	0.710
n	↗	4.996	5.002	5.017	5.100
κ	↗	4.130	4.155	4.220	4.595
ε_1	↘	7.911	7.761	7.364	4.904
ε_2	↗	41.268	41.568	42.350	46.869
For $\mathbf{r_a = r_{Mg}}$,					
$\eta_p \gg 1$	↘	604	241	121	40
E_{gp1} in eV	↘	0.889	0.882	0.864	0.760
n	↗	4.881	4.887	4.902	4.986
κ	↗	3.958	3.983	4.047	4.414
ε_1	↘	8.157	8.019	7.653	5.380
ε_2	↗	38.645	38.933	39.684	44.020
For $\mathbf{r_a = r_{In}}$,					
$\eta_p \gg 1$	↘	603.6	241	120.7	40
E_{gp1} in eV	↘	0.892	0.884	0.866	0.762

n	↗	4.875	4.881	4.897	4.981
κ	↗	3.950	3.975	4.039	4.405
ε_1	↘	8.166	8.029	7.665	5.400
ε_2	↗	38.519	38.806	39.555	43.883
		x=1			
For $\mathbf{r_a} = \mathbf{r_{Ga}}$,					
$\eta_p \gg 1$	↘	565	226	113	37.7
E_{gp1} in eV	↘	0.351	0.346	0.334	0.255
n	↗	5.533	5.536	5.545	5.602
κ	↗	6.018	6.036	6.089	6.430
ε_1	↘	−5.598	−5.786	−6.328	−9.970
ε_2	↗	66.591	66.834	67.531	72.046
For $\mathbf{r_a} = \mathbf{r_{Mg}}$,					
$\eta_p \gg 1$	↘	564	225.7	112.8	37.6
E_{gp1} in eV	↘	0.393	0.389	0.377	0.297
n	↗	5.422	5.425	5.434	5.491
κ	↗	5.839	5.857	5.909	6.245
ε_1	↘	−4.696	−4.874	−5.389	−8.851
ε_2	↗	63.314	63.548	64.223	68.595
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↘	564	225.7	112.8	37.6
E_{gp1} in eV	↘	0.396	0.391	0.379	0.299
n	↗	5.416	5.419	5.429	5.486
κ	↗	5.830	5.848	5.900	6.236
ε_1	↘	−4.654	−4.832	−5.345	−8.799
ε_2	↗	63.154	63.389	64.063	68.427
T in K	↗	20	50	100	300