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OPTICAL COEFFICIENTS IN THE N(P)-TYPE DEGENERATE InSb(1-x)P(x)-CRYSTALLINE ALLOY, DUE TO THE NEW STATIC DIELECTRIC CONSTANT-LAW AND THE GENERALIZED MOTT CRITERIUM IN THE METAL-INSULATOR TRANSITION (22)

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ABTRACT

In the n(p)-type $\mathbf{X(x) \equiv InSb_{1-x}P_x}$- crystalline alloy, with $0 \leq x \leq 1$, basing on our two recent works[1,2], for a given x, and with an increasing $r_{d(a)}$, the optical coefficients have been determined, as functions of the photon energy E, total impurity density N, the donor (acceptor) radius $r_{d(a)}$, concentration x, and temperature T. Those results have been affected by **(i)** the important new $\varepsilon(r_{d(a)}, x)$-law, developed in Equations (8a, 8b), stating that, for a given x, due to the impurity-size effect, ε decreases (↘) 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 $\mathbf{2.86 \times 10^{-7}}$, 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: $InSb_{1-x}P_x$- crystalline alloy; impurity-size effect; Mott critical impurity density in the MIT, optical coefficients.

INTRODUCTION

Here, basing on our two recent works[1, 2] and also other ones[3-8], all the optical coefficients given in the n(p)-type $\mathbf{X(x)} \equiv \mathbf{InSb_{1-x}P_x}$- crystalline alloy, with $0 \leq x \leq 1$, are investigated, as functions of the photon energy E, total impurity density N, the donor (acceptor) radius $r_{d(a)}$, concentration x, and temperature T.

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

ENERGY BAND 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: $\mathbf{r_{do(ao)}}$**=**$\mathbf{r_{Sb(In)}}$**=0.136 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:

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

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

$$\varepsilon_o(x) = 12.5 \times x + 16.8 \times (1 - x). \quad (2)$$

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

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

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

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

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** **$\varepsilon(r_{d(a)}, x)$-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 $\varepsilon(r_{d(a)},x)$-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 $N = N_{CDn(CDp)}(r_{d(a)},x)$: $r_{sn(sp)}(N_{CDn(CDp)}(r_{d(a)},x), r_{d(a)},x) =$ **2.4813963**, for any $(r_{d(a)},x)$-values. So, from Eq. (9b), one also has :

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

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 $\boldsymbol{\mathcal{H}_{n(p)}} = \mathbf{0.47137}$, 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 $\mathbf{2.86 \times 10^{-7}}$. Therefore, the density of electrons (holes) given in parabolic conduction (valence) bands can be defined, as that given in compensated materials, by:

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

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:

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

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 $m_r(x)/m_o$ 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:

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

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

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

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:

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

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

$$\Delta E_{gn}(N, r_d, x) = \Delta E_{gno}(N, r_d, x) \times \{\mathbf{1.2} \times x + \mathbf{0.9} \times (1 - x)\}, \tag{14n}$$

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

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

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

$$\Delta E_{gp}(N, r_a, x) = \Delta E_{gpo}(N, r_a, x) \times \{\mathbf{23} \times x + \mathbf{10} \times (1-x)\}, \quad (14p)$$

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]

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

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 $E \gtrsim E_{gn1(gp1)}$,

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

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

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

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:

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

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

being equal to 0 for $E^* = 0$ (or for $E = E_{gn1(gp1)}$), and also going to 0 as E^{-1} as $E \to \infty$, and further,

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

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: $X_i(E_{gn1(gp1)}) = \frac{A_i}{Q_i} \times \left[-\frac{B_i^2}{2} + E_{gn1(gp1)} B_i - E_{gn1(gp1)}^2 + C_i\right]$, $Y_i(E_{gn1(gp1)}) = \frac{A_i}{Q_i} \times \left[\frac{B_i \times (E_{gn1(gp1)}^2 + C_i)}{2} - 2E_{gn1(gp1)} C_i\right]$, $Q_i = \frac{\sqrt{4C_i - B_i^2}}{2}$, 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 $\mathbf{X(x) \equiv InSb_{1-x}P_x}$- crystalline alloy, as follows.

A. Metal-insulator transition (MIT)-case

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

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 $\eta_{n(p)}(\gg 1$, 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 $\eta_{n(p)}(\gg 1$, 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 $\mathbf{X(x) \equiv InSb_{1-x}P_x}$ –crystalline alloy, by basing on our two recent works[1, 2], for a given x, and with an increasing $r_{d(a)}$, the optical coefficients have been determined, as functions of the photon energy E, total impurity density N, the donor (acceptor) radius $r_{d(a)}$, concentration x, and temperature T.

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

Further, we also showed that $N_{CDn(NDp)}$ is just the density of carriers localized in exponential band tails, with a precision of the order of $\mathbf{2.86 \times 10^{-7}}$, 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	↗	228.55	229.29	230	230.04
n_{MIT}	↘	4.708	4.585	4.490	4.485
$\varepsilon_{1(MIT)}$	↘	22.16	21.02	20.16	20.12
R_{MIT}	↘	0.422	0.412	0.404	0.4037
At **x=0.5**,					
E_{CPE} in meV	↗	825.32	826.2	827	827.04
n_{MIT}	↘	4.167	4.053	3.964	3.959
$\varepsilon_{1(MIT)}$	↘	17.37	16.43	15.71	15.68
R_{MIT}	↘	0.376	0.365	0.3559	0.356
At **x=1**,					
E_{CPE} in meV	↗	1422	1423	1424	1424.05
n_{MIT}	↘	3.614	3.508	3.426	3.422
$\varepsilon_{1(MIT)}$	↘	13.06	12.31	11.74	11.71
R_{MIT}	↘	0.321	0.309	0.300	0.29999
Acceptor		Ga	Mg	In	Cd
r_a (nm)	↗	0.126	0.140	0.144	0.148
At **x=0**,					
E_{CPE} in meV	↗	227.45	229.87	230	230.13
n_{MIT}	↘	4.576	4.494	4.490	4.485
$\varepsilon_{1(MIT)}$	↘	20.94	20.20	20.16	20.12
R_{MIT}	↘	0.411	0.404	0.4041	0.4038
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	↗	1418	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	0.3008	0.3004	0.30002

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

Donor		P	As	Sb	Sn
At **x=0**,					
n_{∞}	↘	2.546	2.424	2.329	2.324
$\varepsilon_{1,\infty}$	↘	6.482	5.875	5.424	5.403
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	11.617	11.060	10.627	10.606
α_{∞} in $(10^9 \times cm^{-1}) = 2.1602$					
R_{∞}	↘	0.190	0.173	0.159	0.1587
At **x=0.5**,					
n_{∞}	↘	2.377	2.263	2.175	2.170
$\varepsilon_{1,\infty}$	↘	5.652	5.123	4.730	4.711
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	10.848	10.329	9.924	9.904
α_{∞} in $(10^9 \times cm^{-1}) = 2.1602$					
R_{∞}	↘	0.166	0.150	0.137	0.136
At **x=1**,					
n_{∞}	↘	2.196	2.091	2.009	2.005
$\varepsilon_{1,\infty}$	↘	4.823	4.372	4.036	4.020
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	10.021	9.540	9.167	9.149
α_{∞} in $(10^9 \times cm^{-1}) = 2.1602$					
R_{∞}	↘	0.140	0.124	0.112	0.1118

Acceptor		Ga	Mg	In	Cd
At **x=0**,					
n_{∞}	↘	2.413	2.333	2.329	2.325
$\varepsilon_{1,\infty}$	↘	5.823	5.443	5.424	5.405
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	11.01	10.64	10.63	10.61
α_{∞} in $(10^9 \times cm^{-1}) = 2.1602$					
R_{∞}	↘	0.171	0.160	0.159	0.1588
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_∞	↘	2.081	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	9.17	9.15
$\propto_\infty$ in $(10^9 \times cm^{-1}) = 2.1602$					
R_∞	↘	0.123	0.113	0.112	0.1119

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,				
$\mathbf{E_{CPE} = 0.2285}$	**4.7079**	**0**	**22.1640**	**0**
2	6.995	0.025	48.928	0.348
2.5	8.537	1.953	69.072	33.352
3	6.999	6.309	9.181	88.320
3.5	4.031	5.573	−14.806	44.930
4	4.374	4.305	0.592	37.660
4.5	5.086	5.937	−9.381	60.395
5	1.697	7.610	−55.038	25.825
5.5	−0.276	5.026	−25.185	−2.777
6	0.176	3.551	−12.578	1.249
…				
$\mathbf{10^{22}}$	**2.5459**	**0**	**6.4818**	**0**
At x=0.5,				
$\mathbf{E_{CPE}}$ **=0.8253**	**4.1675**	**0**	**17.3682**	**0**
2	5.420	0.139	29.355	1.507
2.5	6.523	1.061	41.427	13.852
3	5.870	3.885	19.367	45.607
3.5	4.019	3.725	2.278	29.944
4	4.244	3.051	8.702	25.892
4.5	4.767	4.394	3.420	41.897
5	2.188	5.826	−29.152	25.492
5.5	0.578	3.952	−15.288	4.567

6	0.858	2.854	−7.412	4.897
…				
10^{22}	**2.3774**	**0**	**5.6523**	**0**
At x=1,				
E_{CPE} =1.4220	**3.6143**	**0**	**13.0635**	**0**
2	4.100	0.220	16.765	1.809
2.5	4.830	0.440	23.134	4.250
3	4.780	2.045	18.670	19.557
3.5	3.814	2.248	9.489	17.150
4	3.966	2.012	11.686	15.959
4.5	4.347	3.083	9.389	26.801
5	2.479	4.279	−12.169	21.216
5.5	1.207	3.008	−7.591	7.260
6	1.353	2.234	−3.161	6.045
…				
10^{22}	**2.1961**	**0**	**4.8228**	**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} =0.2274	**4.5756**	**0**	**20.9366**	**0**
2	6.865	0.025	47.126	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**
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} =1.4182	**3.5020**	**0**	**12.2643**	**0**
2	3.992	0.220	15.890	1.759
2.5	4.724	0.443	22.117	4.185
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	15.550
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**
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 $\mathbf{r_d = r_P}$,					
$\eta_n \gg 1$	↗	160.7	231.9	405.1	569.5
E_{gn1} in eV	↗	0.133	0.147	0.212	0.299
n	↘	5.819	5.810	5.765	5.703
κ	↘	6.972	6.911	6.618	6.239
ε_1	↗	−14.741	−14.002	−10.596	−6.401
ε_2	↘	81.147	80.310	76.310	71.172
For $\mathbf{r_d = r_{Sb}}$,					
$\eta_n \gg 1$	↗	160.6	231.9	405.1	569.5

E_{gn1} in eV	↗ 0.183	0.212	0.312	0.428
n	↘ 5.568	5.548	5.477	5.392
κ	↘ 6.748	6.618	6.184	5.697
ε_1	↗ −14.529	−13.017	−8.244	−3.377
ε_2	↘ 75.149	73.430	67.744	61.443
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,				
$\eta_n \gg 1$	↗ 160.6	231.9	405.1	569.5
E_{gn1} in eV	↗ 0.184	0.213	0.314	0.430
n	↘ 5.563	5.542	5.471	5.386
κ	↘ 6.743	6.612	6.175	5.686
ε_1	↗ −14.527	−13.001	−8.204	−3.326
ε_2	↘ 75.028	73.293	67.575	61.255
	x=0.5			
For $\mathbf{r_d} = \mathbf{r_P}$,				
$\eta_n \gg 1$	↗ 173.9	250.9	438.2	616.1
E_{gn1} in eV	↗ 0.696	0.704	0.760	0.841
n	↘ 5.236	5.230	5.185	5.119
κ	↘ 4.646	4.619	4.415	4.125
ε_1	↗ 5.822	6.017	7.399	9.196
ε_2	↘ 48.654	48.310	45.782	42.232
For $\mathbf{r_d} = \mathbf{r_{Sb}}$,				
$\eta_n \gg 1$	↗ 173.8	250.8	438.2	616.06
E_{gn1} in eV	↗ 0.752	0.778	0.873	0.988
n	↘ 4.988	4.968	4.891	4.795
κ	↘ 4.439	4.348	4.014	3.628
ε_1	↗ 5.173	5.777	7.807	9.834
ε_2	↘ 44.291	43.197	39.264	34.792
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,				
$\eta_n \gg 1$	↗ 173.76	250.8	438.2	616.06
E_{gn1} in eV	↗ 0.754	0.779	0.875	0.991
n	↘ 4.983	4.962	4.885	4.788
κ	↘ 4.435	4.342	4.006	3.618
ε_1	↗ 5.158	5.769	7.810	9.840
ε_2	↘ 44.204	43.097	39.138	34.651
	x=1			
For $\mathbf{r_d} = \mathbf{r_P}$,				
$\eta_n \gg 1$	↗ 192.7	278.1	485.7	682.9
E_{gn1} in eV	↗ 1.273	1.281	1.341	1.430
n	↘ 4.568	4.562	4.508	4.426
κ	↘ 2.752	2.731	2.563	2.323
ε_1	↗ 13.300	13.355	13.754	14.197
ε_2	↘ 25.142	24.915	23.104	20.568
For $\mathbf{r_d} = \mathbf{r_{Sb}}$,				
$\eta_n \gg 1$	↗ 192.6	278.0	485.7	682.8
E_{gn1} in eV	↗ 1.336	1.363	1.466	1.592
n	↘ 4.325	4.301	4.206	4.087
κ	↘ 2.577	2.502	2.230	1.917
ε_1	↗ 12.070	12.236	12.720	13.031

ε_2	↘	22.290	21.520	18.748	15.671
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↗	192.58	278.0	485.7	682.8
E_{gn1} in eV	↗	1.337	1.364	1.468	1.595
n	↘	4.320	4.295	4.199	4.080
κ	↘	2.573	2.497	2.222	1.909
ε_1	↗	12.044	12.211	12.696	13.003
ε_2	↘	22.233	21.455	18.666	15.581
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 $\mathbf{r_a} = \mathbf{r_{Ga}}$,								
$\eta_p \gg 1$	↗	152.5		225		400		565
E_{gp1} in eV	↗	0.099		0.109		0.171		0.257
n	↘	5.710		5.703		5.661		5.600
κ	↘	7.128		7.084		6.803		6.420
ε_1	↗	−18.207		−17.650		−14.236		−9.859
ε_2	↘	81.404		80.802		77.022		71.913
For $\mathbf{r_a} = \mathbf{r_{Mg}}$,								
$\eta_p \gg 1$	↗	150.6		223.6		398.9		564.3
E_{gp1} in eV	↗	0.118		0.133		0.207		0.304
n	↘	5.617		5.607		5.555		5.486
κ	↘	7.043		6.973		6.639		6.216
ε_1	↗	−18.051		−17.189		−13.221		−8.533
ε_2	↘	79.125		78.194		73.768		68.205
For $\mathbf{r_a} = \mathbf{r_{In}}$,								
$\eta_p \gg 1$	↗	150.5		223.5		398.8		564.2
E_{gp1} in eV	↗	0.119		0.134		0.209		0.307
n	↘	5.613		5.602		5.550		5.481
κ	↘	7.039		6.968		6.631		6.206
ε_1	↗	−18.044		−17.168		−13.174		−8.471
ε_2	↘	79.013		78.067		73.610		68.025
x=0.5								
For $\mathbf{r_a} = \mathbf{r_{Ga}}$,								
$\eta_p \gg 1$	↗	154.4		234.9		426		606
E_{gp1} in eV		0.6481	↘	0.6477	↗	0.6956		0.7750
n		5.1494	↗	5.1498	↘	5.1121		5.0490
κ		4.8276	↗	4.8293	↘	4.6493		4.3596
ε_1		3.2111	↘	3.1983	↗	4.5176		6.4865
ε_2		49.7188	↗	49.7397	↘	47.5358		44.0228

For $\mathbf{r_a} = \mathbf{r_{Mg}}$,					
$\eta_p \gg 1$	↗	149.8	231.2	423.5	603.7
E_{gp1} in eV	↗	0.669	0.674	0.736	0.827
n	↘	5.058	5.054	5.005	4.932
κ	↘	4.749	4.728	4.500	4.172
ε_1	↗	3.037	3.188	4.805	6.912
ε_2	↘	48.040	47.792	45.043	41.154
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↗	149.5	231.0	423.4	603.6
E_{gp1} in eV	↗	0.670	0.676	0.738	0.830
n	↘	5.054	5.049	5.000	4.926
κ	↘	4.745	4.723	4.492	4.163
ε_1	↗	3.027	3.186	4.817	6.930
ε_2	↘	47.958	47.697	44.922	41.016
			x=1		
For $\mathbf{r_a} = \mathbf{r_{Ga}}$,					
$\eta_p \gg 1$	↗	142.9	238	456.0	658
E_{gp1} in eV	↗	1.275	1.289	1.380	1.501
n	↘	4.452	4.440	4.357	4.245
κ	↘	2.746	2.707	2.456	2.140
ε_1	↗	12.281	12.385	12.958	13.446
ε_2	↘	24.452	24.034	21.401	18.169
For $\mathbf{r_a} = \mathbf{r_{Mg}}$,					
$\eta_p \gg 1$	↗	130.5	228.5	449.2	652.3
E_{gp1} in eV	↗	1.294	1.312	1.416	1.548
n	↘	4.367	4.350	4.256	4.132
κ	↘	2.694	2.642	2.360	2.022
ε_1	↗	11.810	11.942	12.541	12.984
ε_2	↘	23.527	22.989	20.088	16.714
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↗	129.8	227.9	448.8	652
E_{gp1} in eV	↗	1.294	1.313	1.417	1.550
n	↘	4.362	4.346	4.251	4.126
κ	↘	2.691	2.639	2.355	2.017
ε_1	↗	11.787	11.920	12.520	12.960
ε_2	↘	23.482	22.939	20.025	16.645
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 $\mathbf{r_d} = \mathbf{r_P}$,					
$\eta_n \gg 1$	↘	569.5	227.8	113.9	37.95

E_{gn1} in eV	↘	0.299	0.297	0.293	0.263
n	↗	5.703	5.704	5.708	5.729
κ	↗	6.239	6.246	6.266	6.395
ε_1	↘	−6.401	−6.475	−6.688	−8.072
ε_2	↗	71.172	71.266	71.537	73.272
For $\mathbf{r_d} = \mathbf{r_{Sb}}$,					
$\eta_n \gg 1$	↘	569.5	227.8	113.9	37.95
E_{gn1} in eV	↘	0.428	0.426	0.421	0.392
n	↗	5.392	5.394	5.397	5.419
κ	↗	5.697	5.704	5.723	5.846
ε_1	↘	−3.377	−3.440	−3.622	−4.806
ε_2	↗	61.443	61.529	61.775	63.355
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↘	569.5	227.8	113.9	37.946
E_{gn1} in eV	↘	0.430	0.429	0.424	0.394
n	↗	5.386	5.387	5.391	5.412
κ	↗	5.686	5.693	5.712	5.834
ε_1	↘	−3.326	−3.389	−3.570	−4.750
ε_2	↗	61.255	61.340	61.586	63.162
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	↘	0.841	0.840	0.836	0.812
n	↗	5.119	5.121	5.124	5.143
κ	↗	4.125	4.130	4.144	4.228
ε_1	↘	9.196	9.165	9.081	8.576
ε_2	↗	42.232	42.296	42.469	43.495
For $\mathbf{r_d} = \mathbf{r_{Sb}}$,					
$\eta_n \gg 1$	↘	616	246.4	123.2	41.05
E_{gn1} in eV	↘	0.988	0.986	0.982	0.958
n	↗	4.795	4.796	4.800	4.820
κ	↗	3.628	3.633	3.646	3.725
ε_1	↘	9.834	9.811	9.746	9.357
ε_2	↗	34.792	34.849	35.002	35.909
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↘	616	246.4	123.2	41.05
E_{gn1} in eV	↘	0.991	0.989	0.985	0.961
n	↗	4.788	4.790	4.793	4.813
κ	↗	3.618	3.623	3.636	3.715
ε_1	↘	9.840	9.816	9.752	9.365
ε_2	↗	34.651	34.707	34.860	35.764
x=1					
For $\mathbf{r_d} = \mathbf{r_P}$,					
$\eta_n \gg 1$	↘	682.9	273.1	136.6	45.5
E_{gn1} in eV	↘	1.430	1.428	1.425	1.407
n	↗	4.426	4.428	4.431	4.448
κ	↗	2.323	2.327	2.336	2.384
ε_1	↘	14.197	14.191	14.177	14.099

ε_2	↗	20.567	20.606	20.701	21.205
For $\mathbf{r_d} = \mathbf{r_{Sb}}$,					
$\eta_n \gg 1$	↘	682.8	273.1	136.5	45.5
E_{gn1} in eV	↘	1.592	1.590	1.587	1.569
n	↗	4.087	4.089	4.092	4.109
κ	↗	1.917	1.920	1.929	1.972
ε_1	↘	13.031	13.029	13.024	12.995
ε_2	↗	15.671	15.703	15.784	16.208
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↘	682.8	273.1	136.5	45.5
E_{gn1} in eV	↘	1.595	1.594	1.590	1.572
n	↗	4.080	4.081	4.085	4.102
κ	↗	1.909	1.913	1.921	1.964
ε_1	↘	13.003	13.001	12.996	12.968
ε_2	↗	15.581	15.613	15.693	16.115
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 $\eta_p (\gg 1, \text{degenerate case})$, E_{gp1}, n, κ, ε_1 and ε_2, obtained as functions of T, being represented by the arrows: ↗ and ↘, noting that both η_p and E_{gp1} decrease with increasing T.

T in K	↗	20	50	100	300
		x=0			
For $\mathbf{r_a} = \mathbf{r_{Ga}}$,					
$\eta_p \gg 1$	↘	565	226	113	37.7
E_{gp1} in eV	↘	0.257	0.255	0.251	0.221
n	↗	5.600	5.601	5.605	5.626
κ	↗	6.420	6.427	6.448	6.578
ε_1	↘	−9.859	−9.937	−10.162	−11.624
ε_2	↗	71.913	72.008	72.278	74.013
For $\mathbf{r_a} = \mathbf{r_{Mg}}$,					
$\eta_p \gg 1$	↘	564.2	225.7	112.8	37.6
E_{gp1} in eV	↘	0.304	0.303	0.298	0.268
n	↗	5.486	5.488	5.491	5.512
κ	↗	6.216	6.223	6.243	6.371
ε_1	↘	−8.533	−8.607	−8.820	−10.204
ε_2	↗	68.205	68.296	68.557	70.234
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↘	564.2	225.7	112.8	37.59
E_{gp1} in eV	↘	0.307	0.305	0.300	0.271
n	↗	5.481	5.482	5.485	5.506
κ	↗	6.206	6.212	6.233	6.361
ε_1	↘	−8.471	−8.545	−8.758	−10.138
ε_2	↗	68.025	68.116	68.377	70.051
		x=0.5			
For $\mathbf{r_a} = \mathbf{r_{Ga}}$,					

$\eta_p \gg 1$	↘	606	242.4	121	40
E_{gp1} in eV	↘	0.775	0.773	0.769	0.745
n	↗	5.049	5.050	5.053	5.072
κ	↗	4.359	4.365	4.380	4.466
ε_1	↘	6.486	6.451	6.356	5.785
ε_2	↗	44.023	44.088	44.264	45.309
For $\mathbf{r_a} = \mathbf{r_{Mg}}$,					
$\eta_p \gg 1$	↘	604	241.5	120.7	40
E_{gp1} in eV	↘	0.827	0.826	0.822	0.798
n	↗	4.932	4.933	4.936	4.955
κ	↗	4.172	4.178	4.192	4.277
ε_1	↘	6.912	6.880	6.793	6.268
ε_2	↗	41.154	41.217	41.386	42.387
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↘	603.6	241.4	120.7	40.2
E_{gp1} in eV	↘	0.830	0.829	0.825	0.801
n	↗	4.926	4.927	4.930	4.950
κ	↗	4.163	4.169	4.183	4.267
ε_1	↘	6.930	6.898	6.812	6.288
ε_2	↗	41.016	41.079	41.247	42.246
			x=1		
For $\mathbf{r_a} = \mathbf{r_{Ga}}$,					
$\eta_p \gg 1$	↘	658	263.2	131.6	43.85
E_{gp1} in eV	↘	1.501	1.500	1.496	1.478
n	↗	4.245	4.247	4.250	4.267
κ	↗	2.140	2.143	2.152	2.198
ε_1	↘	13.446	13.442	13.432	13.376
ε_2	↗	18.169	18.204	18.292	18.758
For $\mathbf{r_a} = \mathbf{r_{Mg}}$,					
$\eta_p \gg 1$	↘	652	260.9	130.4	43.47
E_{gp1} in eV	↘	1.548	1.547	1.543	1.525
n	↗	4.132	4.133	4.137	4.154
κ	↗	2.022	2.026	2.034	2.079
ε_1	↘	12.984	12.981	12.974	12.931
ε_2	↗	16.714	16.747	16.831	17.272
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↘	652	260.8	130.4	43.45
E_{gp1} in eV	↘	1.550	1.549	1.546	1.528
n	↗	4.126	4.128	4.131	4.148
κ	↗	2.017	2.020	2.029	2.073
ε_1	↘	12.960	12.957	12.950	12.908
ε_2	↗	16.645	16.678	16.761	17.201
T in K	↗	20	50	100	300