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OPTICAL COEFFICIENTS IN THE N(P)-TYPE DEGENERATE InSb(1-x)As(x)-CRYSTALLINE ALLOY, DUE TO THE NEW STATIC DIELECTRIC CONSTANT-LAW AND THE GENERALIZED MOTT CRITERIUM IN THE METAL-INSULATOR TRANSITION (23)

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ABTRACT

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

INTRODUCTION

Here, basing on our two recent works[1,2] and also other ones,[3-8] all the optical coefficients given in the n(p)-type $\mathbf{XX(x) \equiv InSb_{1-x}As_x}$- crystalline alloy, with $0 \le x \le 1$, 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:

$$m_{c(v)}(x)/m_o = 0.09\,(0.3) \times x + 0.1(0.4) \times (1-x) \qquad (1)$$

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

$$\varepsilon_o(x) = 14.55 \times x + 16.8 \times (1-x). \qquad (2)$$

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

$$E_{go}(x) = 0.43 \times x + 0.23 \times (1-x). \qquad (3)$$

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:

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

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

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

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

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

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

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

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 $r_{d(a)} \le r_{do(ao)}$, since $\varepsilon(r_{d(a)}, x) = \frac{\varepsilon_o(x)}{\sqrt{1-\left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3-1\right]\times\ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3}} \ge \varepsilon_o(x)$, 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**,

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

$$a_{Bn(Bp)}(r_{d(a)}, x) \equiv \frac{\varepsilon(r_{d(a)}, x)\times\hbar^2}{m_{c(v)}(x)\times q^2} = 0.53\times10^{-8}\text{ cm}\times\frac{\varepsilon(r_{d(a)}, x)}{m_{c(v)}(x)/m_o}. \quad (8c)$$

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 $\varepsilon(r_{d(a)}, x)$-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:

$$r_{sn(sp)}(N, r_{d(a)}, x) \equiv \left(\frac{3}{4\pi N}\right)^{1/3} \times \frac{1}{a_{Bn(Bp)}(r_{d(a)}, x)} = 1.1723\times10^8\times\left(\frac{1}{N}\right)^{1/3}\times\frac{m_{c(v)}(x)/m_o}{\varepsilon(r_{d(a)}, x)}, \quad (9b)$$

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 :

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

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 $\mathbf{2.86}\times\mathbf{10^{-7}}$. 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 $r_{d(a)}$

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:

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

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

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

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

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

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

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

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:

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

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

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

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:

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

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

$$\Delta E_{gp}(N, r_a, x) = \Delta E_{gpo}(N, r_a, x) \times \{\mathbf{9} \times x + \mathbf{10} \times (1 - x)\}, \quad (14p)$$

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:

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

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

$R(E, N, r_{d(a)}, x, T) = \frac{[n(E)-1]^2 + \kappa(E)^2}{[n(E)+1]^2 + \kappa(E)^2}$. (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 $E_{gni(gpi)} \leq E \leq 2.3$ 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: $X_i(E_{gn1(gp1)}) = \frac{A_i}{Q_i} \times \left[-\frac{B_i^2}{2} + E_{gn1(gp1)} B_i - E_{gn1(gp1)}^2 + C_i\right]$,

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

A. Metal-insulator transition (MIT)-case

As discussed above, the physical conditions used for the MIT are found to be given by: T=0K, $N^* = 0$ 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 $\varepsilon_{1,\infty}(r_{d(a)}, x)$, $\sigma_{0,\infty}(r_{d(a)}, x)$, $\alpha_\infty(r_{d(a)}, x)$ and $R_\infty(r_{d(a)}, x)$ go to their appropriate limiting constants, 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 $\mathbf{X(x)} \equiv \mathbf{InSb_{1-x}As_x}$ –crystalline alloy, by basing on our two recent works[1,2] for a given x, and with an increasing $r_{d(a)}$, the optical coefficients have been determined, as functions of the photon energy E, total impurity density N, the donor (acceptor) radius $r_{d(a)}$, concentration x, and temperature T.

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

Further, we also showed that $N_{CDn(NDp)}$ is just the density of carriers localized in exponential band tails, with a precision of the order of $\mathbf{2.86 \times 10^{-7}}$, 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	↗	328.42	329.22	330	330.04
n_{MIT}	↘	4.559	4.440	4.348	4.344
$\varepsilon_{1(MIT)}$	↘	20.784	19.72	18.91	18.87
R_{MIT}	↘	0.410	0.400	0.3919	0.3915
At **x=1**,					
E_{CPE} in meV	↗	428.27	429.14	430	430.04
n_{MIT}	↘	4.407	4.293	4.204	4.199
$\varepsilon_{1(MIT)}$	↘	19.42	18.43	17.67	17.64
R_{MIT}	↘	0.397	0.387	0.379	0.3786

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	4.486
$\varepsilon_{1(MIT)}$	↘	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	↗	327.4	329.9	330	330.14
n_{MIT}	↘	4.431	4.352	4.348	4.344
$\varepsilon_{1(MIT)}$	↘	19.63	18.94	18.91	18.87
R_{MIT}	↘	0.399	0.392	0.3919	0.3916
At **x=1**,					

E_{CPE} in meV	↗	427.4	429.9	430	430.13
n_{MIT}	↘	4.284	4.208	4.204	4.200
$\varepsilon_{1(MIT)}$	↘	18.35	17.70	17.67	17.64
R_{MIT}	↘	0.386	0.3794	0.3790	0.3787

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_{∞}	↘	2.546	2.424	2.329	2.324
$\varepsilon_{1,\infty}$	↘	6.482	5.875	5.424	5.403
$\sigma_{O,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	11.617	11.060	10.627	10.606
$\propto_{\infty}$ in $(10^9 \times cm^{-1}) = 2.1602$					
R_{∞}	↘	0.190	0.173	0.159	0.1587
At **x=0.5**,					
n_{∞}	↘	2.459	2.341	2.250	2.245
$\varepsilon_{1,\infty}$	↘	6.048	5.482	5.061	5.041
$\sigma_{O,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	11.221	10.684	10.265	10.245
$\propto_{\infty}$ in $(10^9 \times cm^{-1}) = 2.1602$					
R_{∞}	↘	0.178	0.161	0.1479	0.1472
At **x=1**,					
n_{∞}	↘	2.369	2.256	2.167	2.163
$\varepsilon_{1,\infty}$	↘	5.614	5.088	4.698	4.679
$\sigma_{O,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	10.811	10.293	9.890	9.871
$\propto_{\infty}$ in $(10^9 \times cm^{-1}) = 2.1602$					
R_{∞}	↘	0.165	0.149	0.1358	0.1352

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
$\sigma_{O,\infty}$ 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	0.1588
At **x=0.5**,					
n_{∞}	↘	2.331	2.253	2.250	2.246

$\varepsilon_{1,\infty}$	↘	5.433	5.078	5.061	5.043
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	10.63	10.28	10.26	10.25
$\propto_\infty$ in $(10^9\times cm^{-1}) = 2.1602$					
R_∞	↘	0.160	0.148	0.1479	0.1473
At **x=1**,					
n_∞	↘	2.246	2.171	2.167	2.164
$\varepsilon_{1,\infty}$	↘	5.043	4.714	4.698	4.681
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	10.25	9.91	9.89	9.87
$\propto_\infty$ in $(10^9\times cm^{-1}) = 2.1602$					
R_∞	↘	0.147	0.136	0.1358	0.1353

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,				
$\mathbf{E_{CPE}}$ **=0.3284**	**4.5589**	**0**	**20.7837**	**0**
2	6.654	0.042	44.275	0.554
2.5	8.119	1.785	62.725	28.988
3	6.748	5.863	11.163	79.125
3.5	3.983	5.238	−11.568	41.727
4	4.303	4.080	1.864	35.114
4.5	4.980	5.663	−7.261	56.407
5	1.733	7.295	−50.214	25.291

5.5	−0.177	4.837	−23.369	−1.713
6	0.244	3.429	−11.699	1.671
…				
10^{22}	**2.4592**	**0**	**6.0478**	**0**
At x=1,				
E_{CPE} =0.4283	**4.4068**	**0**	**19.4200**	**0**
2	6.318	0.060	39.909	0.759
2.5	7.706	1.625	56.743	25.043
3	6.495	5.433	12.673	70.574
3.5	3.927	4.913	−8.717	38.589
4	4.225	3.861	2.938	32.629
4.5	4.869	5.395	−5.396	52.538
5	1.762	6.987	−45.709	24.617
5.5	−0.087	4.652	−21.637	−0.810
6	0.303	3.309	−10.860	2.007
…				
10^{22}	**2.3693**	**0**	**5.6137**	**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} =0.3274	**4.4311**	**0**	**19.6352**	**0**

2	6.528	0.041	42.615	0.541
2.5	7.993	1.787	60.703	28.568
3	6.621	5.867	9.418	77.696
3.5	3.854	5.241	−12.611	40.403
4	4.174	4.083	0.756	34.083
4.5	4.852	5.665	−8.552	54.982
5	1.604	7.298	−50.691	23.411
5.5	−0.307	4.839	−23.324	−2.974
6	0.114	3.430	−11.753	0.780
…				
10^{22}	**2.3308**	**0**	**5.4328**	**0**
At x=1,				
E_{CPE} =0.4274	**4.2836**	**0**	**18.3495**	**0**
2	6.196	0.060	38.386	0.743
2.5	7.585	1.626	54.887	24.669
3	6.373	5.436	11.061	69.289
3.5	3.803	4.916	−9.701	37.391
4	4.101	3.863	1.894	31.687
4.5	4.746	5.397	−6.607	51.226
5	1.637	6.989	−46.167	22.883
5.5	−0.212	4.654	−21.614	−1.975
6	0.178	3.310	−10.926	1.181
…				
10^{22}	**2.2456**	**0**	**5.0429**	**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 $\mathbf{r_d}$ 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 $\mathbf{r_d} = \mathbf{r_P}$,					
$\eta_n \gg 1$	↗	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 $\mathbf{r_d} = \mathbf{r_{Sb}}$,					
$\eta_n \gg 1$	↗	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 $\mathbf{r_d} = \mathbf{r_P}$,					
$\eta_n \gg 1$	↗	172.1	248.3	433.8	609.8
E_{gn1} in eV	↗	0.202	0.210	0.265	0.345
n	↘	5.685	5.680	5.641	5.583
κ	↘	6.661	6.628	6.387	6.043
ε_1	↗	−12.046	−11.674	−8.976	−5.342
ε_2	↘	75.730	75.293	72.063	67.482
For $\mathbf{r_d} = \mathbf{r_{Sb}}$,					
$\eta_n \gg 1$	↗	172.0	248.3	433.7	609.76
E_{gn1} in eV	↗	0.259	0.284	0.378	0.491
n	↘	5.435	5.418	5.350	5.266
κ	↘	6.412	6.303	5.904	5.439
ε_1	↗	−11.573	−10.375	−6.237	−1.854
ε_2	↘	69.711	68.293	63.173	57.282
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↗	171.98	248.3	433.7	609.77
E_{gn1} in eV	↗	0.260	0.286	0.380	0.494
n	↘	5.430	5.412	5.344	5.259

κ	↘	6.407	6.296	5.894	5.427
ε_1	↗	−11.567	−10.353	−6.190	−1.795
ε_2	↘	69.590	68.154	62.9996	57.085
		x=1			
For $\mathbf{r_d} = \mathbf{r_P}$,					
$\eta_n \gg 1$	↗	185.7	268.0	468.2	658.1
E_{gn1} in eV	↗	0.280	0.285	0.336	0.416
n	↘	5.540	5.537	5.500	5.441
κ	↘	6.319	6.300	6.079	5.744
ε_1	↗	−9.237	−9.036	−6.713	−3.388
ε_2	↘	70.013	69.768	66.874	62.513
For $\mathbf{r_d} = \mathbf{r_{Sb}}$,					
$\eta_n \gg 1$	↗	185.6	267.9	468.1	658.1
E_{gn1} in eV	↗	0.343	0.367	0.462	0.579
n	↘	5.293	5.275	5.206	5.117
κ	↘	6.051	5.949	5.558	5.093
ε_1	↗	−8.598	−7.560	−3.794	0.241
ε_2	↘	64.057	62.768	57.868	52.129
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↗	185.6	267.9	468.1	658.1
E_{gn1} in eV	↗	0.344	0.369	0.464	0.582
n	↘	5.288	5.270	5.199	5.110
κ	↘	6.046	5.942	5.550	5.081
ε_1	↗	−8.588	−7.535	−3.744	0.301
ε_2	↘	63.938	62.630	57.693	51.931
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 $\mathbf{r_a} = \mathbf{r_{Ga}}$,

$\eta_p \gg 1$	↗	163.2	242.4	429	606
E_{gp1} in eV	↗	0.204	0.218	0.292	0.390
n	↘	5.555	5.545	5.493	5.422
κ	↘	6.654	6.591	6.269	5.852
ε_1	↗	−13.416	−12.692	−9.131	−4.850
ε_2	↘	73.936	73.105	68.882	63.462

For $\mathbf{r_a} = \mathbf{r_{Mg}}$,

$\eta_p \gg 1$	↗	164.9	241.0	428	605
E_{gp1} in eV	↗	0.223	0.244	0.330	0.440
n	↘	5.464	5.450	5.388	5.308

κ	↘	6.568	6.479	6.105	5.647
ε_1	↗	−13.278	−12.277	−8.235	−3.716
ε_2	↘	71.782	70.630	65.791	59.953
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↗	163.1	240.9	428	605
E_{gp1} in eV	↗	0.224	0.245	0.332	0.442
n	↘	5.460	5.445	5.383	5.302
κ	↘	6.564	6.474	6.096	5.637
ε_1	↗	−13.272	−12.258	−8.193	−3.664
ε_2	↘	71.676	70.509	65.640	59.783
		x=1			
For $\mathbf{r_a} = \mathbf{r_{Ga}}$,					
$\eta_p \gg 1$	↗	179.6	263	464	655
E_{gp1} in eV	↗	0.304	0.322	0.407	0.517
n	↘	5.399	5.386	5.325	5.243
κ	↘	6.215	6.139	5.784	5.337
ε_1	↗	−9.481	−8.673	−5.103	−1.004
ε_2	↘	67.116	66.130	61.599	55.966
For $\mathbf{r_a} = \mathbf{r_{Mg}}$,					
$\eta_p \gg 1$	↗	178.2	262	463	654
E_{gp1} in eV	↗	0.325	0.350	0.448	0.570
n	↘	5.310	5.292	5.220	5.128
κ	↘	6.126	6.023	5.615	5.128
ε_1	↗	−9.338	−8.272	−4.281	−0.0056
ε_2	↘	65.055	63.749	58.618	52.593
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↗	178.1	262	463	654
E_{gp1} in eV	↗	0.326	0.351	0.450	0.572
n	↘	5.305	5.287	5.214	5.122
κ	↘	6.122	6.017	5.607	5.118
ε_1	↗	−9.332	−8.254	−4.243	0.040
ε_2	↘	65.954	63.633	58.473	52.430
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 $r_d = r_P$,					
$\eta_n \gg 1$	↘	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 $r_d = r_{Sb}$,					
$\eta_n \gg 1$	↘	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 $r_d = r_{Sn}$,					
$\eta_n \gg 1$	↘	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 $r_d = r_P$,					
$\eta_n \gg 1$	↘	609.8	243.9	121.9	40.6
E_{gn1} in eV	↘	0.345	0.343	0.339	0.315
n	↗	5.583	5.585	5.587	5.605
κ	↗	6.043	6.049	6.066	6.168
ε_1	↘	−5.342	−5.407	−5.583	−6.634

ε_2	↗	67.482	67.567	67.794	69.144
For $\mathbf{r_d} = \mathbf{r_{Sb}}$,					
$\eta_n \gg 1$	↘	609.77	243.9	121.9	40.6
E_{gn1} in eV	↘	0.491	0.490	0.486	0.462
n	↗	5.266	5.267	5.270	5.288
κ	↗	5.439	5.445	5.461	5.558
ε_1	↘	−1.854	−1.908	−2.053	−2.928
ε_2	↗	57.282	57.358	57.530	58.779
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↘	609.77	243.9	121.9	40.6
E_{gn1} in eV	↘	0.494	0.493	0.489	0.465
n	↗	5.259	5.260	5.263	5.281
κ	↗	5.427	5.433	5.449	5.546
ε_1	↘	−1.795	−1.849	−1.994	−2.866
ε_2	↗	57.085	57.161	57.366	58.579
x=1					
For $\mathbf{r_d} = \mathbf{r_P}$,					
$\eta_n \gg 1$	↘	658.1	263.2	131.6	43.8
E_{gn1} in eV	↘	0.416	0.415	0.411	0.393
n	↗	5.441	5.442	5.445	5.458
κ	↗	5.744	5.750	5.764	5.839
ε_1	↘	−3.388	−3.443	−3.580	−4.306
ε_2	↗	62.513	62.583	62.772	63.746
For $\mathbf{r_d} = \mathbf{r_{Sb}}$,					
$\eta_n \gg 1$	↘	658.1	263.2	131.6	43.8
E_{gn1} in eV	↘	0.579	0.577	0.574	0.556
n	↗	5.117	5.118	5.121	5.135
κ	↗	5.093	5.099	5.112	5.183
ε_1	↘	0.241	0.197	0.087	−0.500
ε_2	↗	52.129	52.196	52.361	53.229
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↘	658.1	263.2	131.6	43.8
E_{gn1} in eV	↘	0.582	0.581	0.577	0.559

n	↗	5.110	5.111	5.114	5.128
κ	↗	5.081	5.086	5.100	5.170
ε_1	↘	0.301	0.257	0.147	−0.437
ε_2	↗	51.931	51.997	52.161	53.028
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 $\mathbf{r_a = r_{Ga}}$,					
$\eta_p \gg 1$	↘	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 $\mathbf{r_a = r_{Mg}}$,					
$\eta_p \gg 1$	↘	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 $\mathbf{r_a = r_{In}}$,					
$\eta_p \gg 1$	↘	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	121.2	40.4
E_{gp1} in eV	↘	0.390	0.389	0.385	0.361
n	↗	5.422	5.423	5.426	5.443
κ	↗	5.852	5.858	5.875	5.975
ε_1	↘	−4.840	−4.912	−5.078	− 6.075
ε_2	↗	63.462	63.543	63.762	65.056

For $\mathbf{r_a} = \mathbf{r_{Mg}}$,

$\eta_p \gg 1$	↘	605	242.0	121.0	40.3
E_{gp1} in eV	↘	0.440	0.438	0.434	0.410
n	↗	5.308	5.309	5.312	5.330
κ	↗	5.647	5.653	5.670	5.768
ε_1	↘	−3.716	−3.774	−3.931	− 4.868
ε_2	↗	59.953	60.031	60.242	61.490

For $\mathbf{r_a} = \mathbf{r_{In}}$,

$\eta_p \gg 1$	↘	605	242.0	121.0	40.3
E_{gp1} in eV	↘	0.442	0.441	0.437	0.413
n	↗	5.302	5.303	5.306	5.324
κ	↗	5.637	5.643	5.660	5.758
ε_1	↘	−3.664	−3.722	−3.878	− 4.812
ε_2	↗	59.782	59.861	60.071	61.317

x=1

For $\mathbf{r_a} = \mathbf{r_{Ga}}$,

$\eta_p \gg 1$	↘	655	262	131	43.6
E_{gp1} in eV	↘	0.517	0.515	0.512	0.494
n	↗	5.243	5.244	5.246	5.260
κ	↗	5.337	5.343	5.357	5.429
ε_1	↘	−1.004	−1.052	−1.172	− 1.810
ε_2	↗	55.966	56.036	56.203	57.117

For $\mathbf{r_a} = \mathbf{r_{Mg}}$,

$\eta_p \gg 1$	↘	654.2	261.7	130.8	43.6
E_{gp1} in eV	↘	0.570	0.568	0.565	0.547
n	↗	5.128	5.129	5.131	5.145

κ	↗	5.128	5.134	5.147	5.218
ε_1	↘	-0.0056	-0.050	-0.162	-0.756
ε_2	↗	52.593	52.660	52.826	53.699
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For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↘	654.2	261.66	130.83	43.592
E_{gp1} in eV	↘	0.572	0.571	0.568	0.549
n	↗	5.122	5.123	5.126	5.139
κ	↗	5.118	5.123	5.137	5.208
ε_1	↘	0.0399	0.0048	-0.116	-0.708
ε_2	↗	52.430	52.497	52.662	53.534
T in K	↗	20	50	100	300