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OPTICAL COEFFICIENTS IN THE N(P)-TYPE DEGENERATE InP(1-x) As(x)-CRYSTALLINE ALLOY, DUE TO THE NEW STATIC DIELECTRIC CONSTANT-LAW AND THE GENERALIZED MOTT CRITERIUM IN THE METAL-INSULATOR TRANSITION (20)

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ABTRACT

In the n(p)-type $\mathbf{X(x) \equiv InP_{1-x}As_x}$- 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 $\mathbf{2.77 \times 10^{-7}}$, 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: $InP_{1-x}As_x$- 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 $\mathbf{X(x)} \equiv \mathbf{InP_{1-x}As_x}$- crystalline alloy, with $0 \leq x \leq 1$, are investigated, as functions of the photon energy E, total impurity density N, the donor (acceptor) radius $r_{d(a)}$, concentration x, and temperature T.

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

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

$$m_{c(v)}(x)/m_o = 0.09\ (0.3) \times x + 0.077(0.5) \times (1 - x) \quad (1)$$

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

$$\varepsilon_o(x) = 14.55 \times x + 12.5 \times (1 - x). \quad (2)$$

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

$$E_{go}(x) = 0.43 \times x + 1.424 \times (1 - x). \quad (3)$$

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

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

and then, the isothermal bulk modulus, by:

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

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

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

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

Furthermore, we also shown that, as $r_{d(a)} > r_{do(ao)}$ $(r_{d(a)} < r_{do(ao)})$, the compression (dilatation) gives rise to the increase (the decrease) in the energy gap $E_{gn(gp)}(r_{d(a)}, x)$, and the effective donor (acceptor)-ionization energy $E_{d(a)}(r_{d(a)}, x)$ in absolute values, obtained in the effective Bohr model, which is represented respectively by: $\pm[\Delta\sigma(r_{d(a)}, x)]_{n(p)}$,

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

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

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

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

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

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

Furthermore, by using $\mathbf{M_{n(p)}} = \mathbf{0.25}$, 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 $\mathbf{2.77 \times 10^{-7}}$. 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:

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

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:

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

where u is the reduced electron density, $u(N, r_{d(a)}, x, T) \equiv \frac{N^*}{N_{c(v)}(T,x)}$, $F(u) = au^{\frac{2}{3}}\left(1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}}\right)^{-\frac{2}{3}}$, $a = \left[(3\sqrt{\pi}/4) \times u\right]^{2/3}$, $b = \frac{1}{8}\left(\frac{\pi}{a}\right)^2$, $c = \frac{62.3739855}{1920}\left(\frac{\pi}{a}\right)^4$, and $G(u) \simeq Ln(u) + 2^{-\frac{3}{2}} \times u \times e^{-du}$; $d = 2^{3/2}\left[\frac{1}{\sqrt{27}} - \frac{3}{16}\right] > 0$. Therefore, from Eq. (12), the Fermi energies are expressed as functions of variables : $N, r_{d(a)}, x$, and T.

Here, one notes that: (i) as $u \gg 1$, according to the HD [d(a)- X(x)- alloy] ER-case, or to the degenerate case, Eq. (12) is reduced to the function F(u), and in particular at T=0 and as $N^* = 0$, according to the metal-insulator transition (**MIT**), one has: $+E_{Fn}(-E_{Fp}) = \frac{\hbar^2}{2\times m_r(x)} \times (3\pi^2 N^*)^{2/3} = 0$, and (ii) $\frac{E_{Fn}(u\ll1)}{k_B T}\left(\frac{-E_{Fp}(u\ll1)}{k_B T}\right) \ll -1$, 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:

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

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

$$\Delta E_{gn}(N, r_d, x) = \Delta E_{gno}(N, r_d, x) \times \{1.25 \times x + 1.3 \times (1 - x)\}, \quad (14n)$$

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 $\mathbf{X(x) \equiv InP_{1-x}As_x}$- 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 $\varepsilon_{1,\infty}(r_{d(a)}, x)$, $\sigma_{O,\infty}(r_{d(a)}, x)$, $\alpha_\infty(r_{d(a)}, x)$ 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 $\mathbf{X(x) \equiv InP_{1-x}As_x}$- 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 $\mathbf{2.77 \times 10^{-7}}$, 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	↗	927	927.3	930	932
n_{MIT}	↘	3.816	3.791	3.592	3.536
$\varepsilon_{1(MIT)}$	↘	14.56	14.37	12.90	12.50
R_{MIT}	↘	0.342	0.339	0.319	0.312
At **x=1**,					
E_{CPE} in meV	↗	430	430.3	433.3	434.4
n_{MIT}	↘	4.204	4.178	3.972	3.913
$\varepsilon_{1(MIT)}$	↘	17.67	17.45	15.77	15.31
R_{MIT}	↘	0.379	0.377	0.357	0.351

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	↗	923.07	926.80	927	927.2
n_{MIT}	↘	3.894	3.820	3.816	3.812
$\varepsilon_{1(MIT)}$	↘	15.16	14.59	14.56	14.53
R_{MIT}	↘	0.350	0.342	0.3419	0.3415
At **x=1**,					
E_{CPE} in meV	↗	427.45	429.87	430	430.1
n_{MIT}	↘	4.284	4.208	4.204	4.200
$\varepsilon_{1(MIT)}$	↘	18.349	17.70	17.67	17.64
R_{MIT}	↘	0.386	0.3791	0.379	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_{∞}	↘	2.009	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_∞	↘	2.090	2.065	1.868	1.812
$\varepsilon_{1,\infty}$	↘	4.367	4.263	3.489	3.284
$\sigma_{O,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	9.535	9.421	8.523	8.269
$\propto_\infty$ in $(10^9 \times cm^{-1}) = 2.1602$					
R_∞	↘	0.124	0.121	0.091	0.083
At **x=1**,					
n_∞	↘	2.167	2.141	1.937	1.880
$\varepsilon_{1,\infty}$	↘	4.698	4.586	3.753	3.533
$\sigma_{O,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	9.890	9.772	8.840	8.577
$\propto_\infty$ in $(10^9 \times cm^{-1}) = 2.1602$					
R_∞	↘	0.136	0.132	0.102	0.093

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_∞	↘	2.165	2.093	2.090	2.086
$\varepsilon_{1,\infty}$	↘	4.688	4.382	4.367	4.351
$\sigma_{O,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	9.879	9.552	9.535	9.519
$\propto_\infty$ in $(10^9 \times cm^{-1}) = 2.1602$					
R_∞	↘	0.135	0.125	0.124	0.1238
At **x=1**,					
n_∞	↘	2.246	2.171	2.167	2.164
$\varepsilon_{1,\infty}$	↘	5.043	4.714	4.698	4.681
$\sigma_{O,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	10.25	9.907	9.890	9.873
$\propto_\infty$ in $(10^9 \times cm^{-1}) = 2.1602$					
R_∞	↘	0.147	0.136	0.136	0.135

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} =0.927	**3.8164**	**0**	**14.5648**	**0**
2	4.919	0.158	24.173	1.556
2.5	5.954	0.937	34.577	11.155
3	5.424	3.530	16.958	38.292
3.5	3.740	3.447	2.105	25.786
4	3.949	2.858	7.425	22.576
4.5	4.445	4.154	2.501	36.933
5	1.994	5.545	−26.776	22.113
5.5	0.443	3.782	−14.110	3.352
6	0.697	2.743	−7.040	3.827
…				
10^{22}	**2.0897**	**0**	**4.3668**	**0**
At x=1,				
E_{CPE} =0.43	**4.2038**	**0**	**17.6721**	**0**
2	6.111	0.060	37.347	0.739
2.5	7.499	1.622	55.598	24.328
3	6.290	5.425	10.135	68.258
3.5	3.726	4.908	−10.204	36.569
4	4.023	3.858	1.303	31.041
4.5	4.667	5.390	−7.276	50.313
5	1.562	6.981	−46.299	21.807
5.5	−0.256	4.649	−21.534	−2.658
6	0.104	3.307	−10.927	0.687
…				
10^{22}	**2.1674**	**0**	**4.6977**	**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} =0.9231	**3.8943**	**0**	**12.1653**	**0**
2	5.002	0.157	25.001	1.575
2.5	6.040	0.941	35.601	11.373
3	5.505	3.543	17.754	39.015
3.5	3.815	3.458	2.600	26.385
4	4.025	2.866	7.987	23.068
4.5	4.522	4.163	3.114	37.654

5	2.066	5.556	−26.603	22.954
5.5	0.513	3.789	−14.093	3.885
6	0.768	2.748	−6.960	4.221
…				
10^{22}	**2.1651**	**0**	**4.6877**	**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 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 $\mathbf{r_d = r_P}$,					
$\eta_n \gg 1$	↗	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 $\mathbf{r_d = r_{Sb}}$,					
$\eta_n \gg 1$	↗	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 $\mathbf{r_d = r_{Sn}}$,					
$\eta_n \gg 1$	↗	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 $\mathbf{r_d = r_P}$,					
$\eta_n \gg 1$	↗	186	268	469	659

E_{gn1} in eV	↗	0.807	0.823	0.900	1.003
n	↘	4.859	4.846	4.783	4.697
κ	↘	4.245	4.189	3.920	3.578
ε_1	↗	5.592	5.942	7.509	9.264
ε_2	↘	41.260	40.604	37.503	33.611
For $\mathbf{r_d} = \mathbf{r_{Sb}}$,					
$\eta_n \gg 1$	↗	185.8	268	469	659
E_{gn1} in eV	↗	0.875	0.913	1.040	1.180
n	↘	4.582	4.551	4.447	4.323
κ	↘	4.007	3.879	3.469	3.026
ε_1	↗	4.940	5.669	7.743	9.537
ε_2	↘	36.721	33.306	30.849	26.161
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↗	185.7	268	469	659
E_{gn1} in eV	↗	0.891	0.933	1.069	1.180
n	↘	4.513	4.478	4.447	4.364
κ	↘	3.952	3.808	3.469	3.367
ε_1	↗	4.750	5.552	7.743	7.705
ε_2	↘	35.675	34.106	30.849	29.390
		x=1			
For $\mathbf{r_d} = \mathbf{r_P}$,					
$\eta_n \gg 1$	↗	185.6	267.9	468	658
E_{gn1} in eV	↗	0.325	0.345	0.429	0.537
n	↘	5.306	5.292	5.230	5.149
κ	↘	6.126	6.044	5.692	5.257
ε_1	↗	−9.372	−8.523	−5.050	−1.121
ε_2	↘	65.002	63.965	59.545	54.134
For $\mathbf{r_d} = \mathbf{r_{Sb}}$,					
$\eta_n \gg 1$	↗	185.4	267.8	468	658
E_{gn1} in eV	↗	0.392	0.433	0.563	0.711
n	↘	5.027	4.997	4.899	4.784
κ	↘	5.843	5.676	5.154	4.594
ε_1	↗	−8.870	−7.244	−2.566	1.786
ε_2	↘	58.745	56.725	50.503	43.957
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↗	185.3	267.7	467.9	657.9
E_{gn1} in eV	↗	0.408	0.454	0.594	0.751
n	↘	4.958	4.924	4.817	4.694
κ	↘	5.778	5.591	5.033	4.446
ε_1	↗	−8.804	−7.019	−2.121	2.272
ε_2	↘	57.287	55.065	48.488	41.741
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 $\mathbf{r_a = r_{Ga}}$,					
$\eta_p \gg 1$	↗	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 $\mathbf{r_a = r_{Mg}}$,					
$\eta_p \gg 1$	↗	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 $\mathbf{r_a = r_{In}}$,					
$\eta_p \gg 1$	↗	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 $\mathbf{r_a = r_{Ga}}$,					
$\eta_p \gg 1$	↗	167.6	253	458	650
E_{gp1} in eV	↗	0.771	0.782	0.856	0.959
n	↘	4.964	4.955	4.895	4.809
κ	↘	4.374	4.334	4.072	3.721
ε_1	↗	5.506	5.766	7.375	9.281
ε_2	↘	43.430	42.955	39.869	35.796
For $\mathbf{r_a = r_{Mg}}$,					
$\eta_p \gg 1$	↗	163.2	249.9	455	648
E_{gp1} in eV	↗	0.791	0.809	0.897	1.012
n	↘	4.876	4.862	4.790	4.693
κ	↘	4.300	4.239	3.933	3.549
ε_1	↗	5.278	5.665	7.474	9.432
ε_2	↘	41.935	41.220	37.675	33.314
For $\mathbf{r_a = r_{In}}$,					
$\eta_p \gg 1$	↗	163	249.7	455	647.6
E_{gp1} in eV	↗	0.792	0.810	0.899	1.014
n	↘	4.871	4.857	4.784	4.687
κ	↘	4.297	4.235	3.926	3.541
ε_1	↗	5.266	5.659	7.478	9.437

ε_2	↘	41.862	41.136	37.568	33.195
		x=1			
For $\mathbf{r_a} = \mathbf{r_{Ga}}$,					
$\eta_p \gg 1$	↗	179.6	263	464	654.9
E_{gp1} in eV	↗	0.303	0.322	0.406	0.516
n	↘	5.399	5.387	5.325	5.243
κ	↘	6.218	6.141	5.787	5.340
ε_1	↗	−9.509	−8.700	−5.128	−1.025
ε_2	↘	67.150	66.163	61.631	55.997
For $\mathbf{r_a} = \mathbf{r_{Mg}}$,					
$\eta_p \gg 1$	↗	178.2	262	463.5	654.2
E_{gp1} in eV	↗	0.325	0.349	0.447	0.569
n	↘	5.310	5.292	5.220	5.128
κ	↘	6.129	6.026	5.617	5.131
ε_1	↗	−9.366	−8.299	−4.304	−0.025
ε_2	↘	65.088	63.782	58.649	52.623
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↗	178.1	261.8	463.4	654.17
E_{gp1} in eV	↗	0.326	0.350	0.449	0.572
n	↘	5.305	5.288	5.215	5.122
κ	↘	6.124	6.020	5.609	5.120
ε_1	↗	−9.359	−8.280	−4.266	0.020
ε_2	↘	64.987	63.666	58.504	52.460
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 $\mathbf{r_d} = \mathbf{r_P}$,					
$\eta_n \gg 1$	↘	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 $\mathbf{r_d} = \mathbf{r_{Sb}}$,					
$\eta_n \gg 1$	↘	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 $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↘	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 $\mathbf{r_d} = \mathbf{r_P}$,					
$\eta_n \gg 1$	↘	659	263.8	131.9	43.95
E_{gn1} in eV	↘	1.003	0.996	0.977	0.874
n	↗	4.692	4.703	4.719	4.805
κ	↗	3.578	3.601	3.662	4.011
ε_1	↘	9.264	9.152	8.857	6.998
ε_2	↗	33.611	33.875	34.563	38.548
For $\mathbf{r_d} = \mathbf{r_{Sb}}$,					
$\eta_n \gg 1$	↘	659	263.7	131.9	43.94
E_{gn1} in eV	↘	1.180	1.172	1.154	1.050
n	↗	4.323	4.330	4.346	4.435
κ	↗	3.026	3.047	3.103	3.425
ε_1	↘	9.537	9.460	9.256	7.939
ε_2	↗	26.161	26.386	26.973	30.384
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↘	659	263.7	131.9	43.94
E_{gn1} in eV	↘	1.221	1.214	1.195	1.091
n	↗	4.231	4.238	4.254	4.344
κ	↗	2.904	2.925	2.980	3.295
ε_1	↘	9.473	9.404	9.218	8.012
ε_2	↗	24.574	24.790	25.353	28.633
			x=1		
For $\mathbf{r_d} = \mathbf{r_P}$,					
$\eta_n \gg 1$	↘	658	263.2	131.6	43.85
E_{gn1} in eV	↘	0.537	0.533	0.520	0.441
n	↗	5.149	5.152	5.162	5.221
κ	↗	5.257	5.274	5.323	5.643
ε_1	↘	−1.121	−1.269	−1.696	−4.580
ε_2	↗	54.134	54.347	54.958	58.923
For $\mathbf{r_d} = \mathbf{r_{Sb}}$,					
$\eta_n \gg 1$	↘	658	263.2	131.6	43.85
E_{gn1} in eV	↘	0.711	0.706	0.694	0.615
n	↗	4.784	4.788	4.798	4.859
κ	↗	4.594	4.610	4.656	4.955
ε_1	↘	1.786	1.671	1.336	−0.939
ε_2	↗	43.957	44.143	44.678	48.159
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↘	658	263.1	131.6	43.84
E_{gn1} in eV	↘	0.751	0.747	0.734	0.655
n	↗	4.694	4.698	4.708	4.770
κ	↗	4.446	4.462	4.507	4.801

ε_1	↘	2.272	2.163	1.848	−0.297
ε_2	↗	41.741	41.921	42.439	45.808
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 $\mathbf{r_a = r_{Ga}}$,					
$\eta_p \gg 1$	↘	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 $\mathbf{r_a = r_{Ga}}$,					
$\eta_p \gg 1$	↘	650	260	130	43.3
E_{gp1} in eV	↘	0.959	0.952	0.934	0.830
n	↗	4.809	4.815	4.831	4.916
κ	↗	3.721	3.745	3.807	4.163
ε_1	↘	9.281	9.160	8.840	6.834
ε_2	↗	35.796	36.071	36.788	40.935
For $\mathbf{r_a = r_{Mg}}$,					
$\eta_p \gg 1$	↘	647.8	259	129	43.2
E_{gp1} in eV	↘	1.012	1.005	0.986	0.883
n	↗	4.693	4.699	4.715	4.801
κ	↗	3.549	3.572	3.633	3.981
ε_1	↘	9.432	9.322	9.032	7.205
ε_2	↗	33.314	33.577	34.262	38.227
For $\mathbf{r_a = r_{In}}$,					

$\eta_p \gg 1$	↘	647.6	259	129	43.1
E_{gp1} in eV	↘	1.014	1.007	0.989	0.885
n	↗	4.687	4.694	4.709	4.796
κ	↗	3.541	3.564	3.625	3.972
ε_1	↘	9.437	9.328	9.039	7.220
ε_2	↗	33.195	33.457	34.140	38.097
			x=1		
For $\mathbf{r_a = r_{Ga}}$,					
$\eta_p \gg 1$	↘	655	262	131	43.6
E_{gp1} in eV	↘	0.516	0.512	0.499	0.420
n	↗	5.243	5.246	5.256	5.315
κ	↗	5.340	5.357	5.407	5.729
ε_1	↘	−1.025	−1.176	−1.615	−4.573
ε_2	↗	55.997	56.214	56.840	60.898
For $\mathbf{r_a = r_{Mg}}$,					
$\eta_p \gg 1$	↘	654	261.7	130.8	43.59
E_{gp1} in eV	↘	0.569	0.565	0.552	0.473
n	↗	5.128	5.131	5.141	5.201
κ	↗	5.131	5.148	5.197	5.512
ε_1	↘	−0.025	−0.166	−0.574	−3.334
ε_2	↗	52.623	52.832	53.434	57.337
For $\mathbf{r_a = r_{In}}$,					
$\eta_p \gg 1$	↘	654	261.66	130.8	43.59
E_{gp1} in eV	↘	0.572	0.567	0.555	0.476
n	↗	5.122	5.126	5.135	5.195
κ	↗	5.120	5.137	5.186	5.501
ε_1	↘	0.020	−0.120	−0.527	−3.277
ε_2	↗	52.460	52.669	53.269	57.164
T in K	↗	20	50	100	300