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OPTICAL COEFFICIENTS IN THE N(P)-TYPE DEGENERATE GaAs(1-x) P(x)-CRYSTALLINE ALLOY, DUE TO THE NEW STATIC DIELECTRIC CONSTANT-LAW AND THE GENERALIZED MOTT CRITERIUM IN THE METAL-INSULATOR TRANSITION. (3)

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ABTRACT

In the n(p)-type $GaAs_{1-x}P_x$- 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, 2.92×10^{-7}, as that given in Table 4 of Ref.[1], according to a definition of the effective density of electrons (holes) given in parabolic conduction (valence) bands by: $N^*(N, r_{d(a)}, x) \equiv N - N_{CDn(NDp)}(r_{d(a)}, x)$, as defined in Eq. (9d). In summary, due to the new $\varepsilon(r_{d(a)}, x)$-law and to the effective density of electrons (holes) given in parabolic conduction (valence) bands $N^*(N, r_{d(a)}, x)$, for a given x, and with an increasing $r_{d(a)}$, the numerical results of all the optical coefficients, obtained in appropriated physical conditions (E, N, T), and

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

KEYWORS: $GaAs_{1-x}P_x$- 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 $X(x) \equiv GaAs_{1-x}P_x$- 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: $r_{do(ao)}$=$r_{As(Ga)}$=0.118 nm (0.126 nm).

A. Effect of x- concentration

Here, the intrinsic energy-band-structure parameters[1], are expressed as functions of x, are given in the following.

(i)-The unperturbed relative effective electron (hole) mass in conduction (valence) bands are given by.

$$m_{c(v)}(x)/m_o = 0.13(0.5) \times x + 0.066\ (0.291) \times (1-x) \quad (1)$$

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

$$\varepsilon_o(x) = 11.1 \times x + 13.13 \times (1-x). \quad (2)$$

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

$$E_{go}(x) = 1.796 \times x + 1.52 \times (1-x). \quad (3)$$

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:

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

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

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

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

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

corresponding to the decrease in both $E_{gn(gp)}(r_{d(a)},x)$ and $E_{d(a)}(r_{d(a)},x)$, with decreasing 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, 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 $N=N_{CDn(CDp)}(r_{d(a)},x)$: $r_{sn(sp)}(N_{CDn(CDp)}(r_{d(a)},x), r_{d(a)},x)=$ **2.4814**, for any $(r_{d(a)},x)$-values. So, from Eq. (9b), one also has.

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

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 $\boldsymbol{\mathcal{H}_{n(p)} = 0.47137}$, 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 $\mathbf{2.92 \times 10^{-7}}$. 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 $r_{d(a)}$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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.

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

$$, N_r \equiv \left(\frac{N^*}{N_{CDn}(r_d, x)}\right), \quad (14n)$$

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

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

$$, N_r \equiv \left(\frac{N^*}{N_{CDp}(r_a, x)}\right), \quad (14p)$$

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

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]

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

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.

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

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

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

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

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

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, $n(E, N, r_{d(a)}, x, T) = n_\infty(r_{d(a)}, x) + \sum_{i=1}^{4} \frac{X_i(E_{gn1(gp1)}) \times E + Y_i(E_{gn1(gp1)})}{E^2 - B_i E + C_i}$. (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 $X(x) \equiv GaAs_{1-x}P_x$- 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 $\alpha_{MIT}(r_{d(a)}, x) = 0$, and the other functions such as : $n_{MIT}(r_{d(a)},x)$ from Eq. (21), and $\varepsilon_{1(MIT)}(r_{d(a)},x)$ and $R_{MIT}(r_{d(a)},x)$ from Eq.(16) decrease with increasing $r_{d(a)}$ and E_{CPE}, as those investigated in Table 1 in Appendix 1.

B. Optical coefficients, obtained as $E \to \infty$

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 $R_{\infty}(r_{d(a)},x)$ Z go to their appropriate limiting constants, as those investigated in Table 2 in Appendix 1.

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

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

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

In the X(x)-system, at E=3.2 eV and T=20 K, for given $r_{d(a)}$ and x, and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of $\eta_{n(p)}(\gg 1$, 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 $N = 10^{20}\text{cm}^{-3}$, 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 $X(x) \equiv GaAs_{1-x}P_x$- 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 2.92×10^{-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	Te	Sb	Sn
r_d (nm) [4]	↗	0.110	0.118	0.132	0.136	0.140
At **x=0**,						
E_{CPE} in meV	↗	1519.8	1520	1520.7	1521.2	1521.8
n_{MIT}	↘	3.437	3.416	3.352	3.313	3.268
$\varepsilon_{1(MIT)}$	↘	11.81	11.67	11.23	10.98	10.68
R_{MIT}	↘	0.302	0.299	0.292	0.288	0.282
At **x=0.5**,						
E_{CPE} in meV	↗	1657.6	1658	1659	1660	1662
n_{MIT}	↘	3.269	3.249	3.187	3.149	3.106
$\varepsilon_{1(MIT)}$	↘	10.69	10.55	10.16	9.92	9.65
R_{MIT}	↘	0.282	0.280	0.273	0.268	0.263
At **x=1**,						
E_{CPE} in meV	↗	1795.4	1796	1798	1799	1801
n_{MIT}	↘	3.098	3.078	3.018	2.982	2.940
$\varepsilon_{1(MIT)}$	↘	9.598	9.476	9.110	8.893	8.646
R_{MIT}	↘	0.262	0.260	0.252	0.248	0.242

Acceptor		B	Ga	Mg	In	Cd
r_a (nm)	↗	0.088	0.126	0.140	0.144	0.148
At **x=0**,						
E_{CPE} in meV	↗	1503.7	1520	1523	1524	1527
n_{MIT}	↘	4.173	3.416	3.358	3.323	3.281
$\varepsilon_{1(MIT)}$	↘	17.41	11.67	11.276	11.04	10.77
R_{MIT}	↘	0.376	0.299	0.293	0.289	0.284
At **x=0.5**,						
E_{CPE} in meV	↗	1632	1658	1662	1665	1669
n_{MIT}	↘	3.982	3.249	3.192	3.157	3.117
$\varepsilon_{1(MIT)}$	↘	15.86	10.55	10.19	9.97	9.71
R_{MIT}	↘	0.358	0.280	0.273	0.269	0.264
At **x=1**,						
E_{CPE} in meV	↗	1757	1796	1802	1807	1812
n_{MIT}	↘	3.789	3.078	3.022	2.988	2.948
$\varepsilon_{1(MIT)}$	↘	14.36	9.47	9.13	8.93	8.69
R_{MIT}	↘	0.339	0.260	0.253	0.248	0.243

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

Donor		P	As	Te	Sb	Sn
At **x=0**,						
n_{∞}	↘	2.08	2.0589	1.9950	1.9566	1.9124
$\varepsilon_{1,\infty}$	↘	4.327	4.2392	3.9800	3.8284	3.6571
$\sigma_{0,\infty}$	in $\frac{10^5}{\Omega \times cm}$ ↘	9.4915	9.3951	9.1033	8.9282	8.7263
α_{∞}	in $(10^9 \times cm^{-1})$	2.160	2.160	2.160	2.160	2.160
R_{∞}	↘	0.123	0.120	0.110	0.105	0.098
At **x=0.5**,						
n_{∞}	↘	1.998	1.978	1.916	1.879	1.837
$\varepsilon_{1,\infty}$	↘	3.992	3.911	3.672	3.532	3.374
$\sigma_{0,\infty}$	in $\frac{10^5}{\Omega \times cm}$ ↘	9.117	9.025	8.744	8.576	8.382
α_{∞}	in $(10^9 \times cm^{-1})$	2.160	2.160	2.160	2.160	2.160
R_{∞}	↘	0.111	0.108	0.099	0.093	0.087
At **x=1**,						
n_{∞}	↘	1.912	1.893	1.834	1.799	1.758
$\varepsilon_{1,\infty}$	↘	3.658	3.584	3.365	3.236	3.092
$\sigma_{0,\infty}$	in $\frac{10^5}{\Omega \times cm}$ ↘	8.727	8.638	8.370	8.209	8.023
α_{∞}	in $(10^9 \times cm^{-1})$	2.160	2.160	2.160	2.160	2.160
R_{∞}	↘	0.098	0.095	0.087	0.081	0.075
Acceptor		**B**	**Ga**	**Mg**	**In**	**Cd**
At **x=0**,						
n_{∞}	↘	2.806	2.059	2.002	1.968	1.928
$\varepsilon_{1,\infty}$	↘	7.872	4.239	4.010	3.874	3.719
$\sigma_{0,\infty}$	in $\frac{10^5}{\Omega \times cm}$ ↘	12.80	9.395	9.138	8.981	8.799
α_{∞}	in $(10^9 \times cm^{-1})$	2.160	2.160	2.160	2.160	2.160
R_{∞}	↘	0.225	0.120	0.111	0.106	0.100
At **x=0.5**,						
n_{∞}	↘	2.695	1.978	1.923	1.891	1.852
$\varepsilon_{1,\infty}$	↘	7.263	3.911	3.700	3.575	3.431
$\sigma_{0,\infty}$	in $\frac{10^5}{\Omega \times cm}$ ↘	12.30	9.025	8.777	8.627	8.452
α_{∞}	in $(10^9 \times cm^{-1})$	2.160	2.160	2.160	2.160	2.160
R_{∞}	↘	0.210	0.108	0.100	0.095	0.089
At **x=1**,						
n_{∞}	↘	2.580	1.893	1.841	1.810	1.773
$\varepsilon_{1,\infty}$	↘	6.655	3.584	3.390	3.275	3.144
$\sigma_{0,\infty}$	in $\frac{10^5}{\Omega \times cm}$ ↘	11.77	8.64	8.402	8.258	8.090
α_{∞}	in $(10^9 \times cm^{-1})$	2.160	2.160	2.160	2.160	2.160
R_{∞}	↘	0.195	0.095	0.088	0.083	0.078

Table 3n: In the P-X(x)-system, 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 $E\ [\geq E_{CPE}(r_p, x)]$ of and x, noting that (i) K=0 and $\varepsilon_2 = 0$ at, $E = E_{CPE}(r_p, x)$ and $\kappa \to 0$ and $E \to \infty$ as.

E in eV	n	κ	ε_1	ε_2
At x=0,				
E_{CPE} = 1.5198	**3.437**	**0**	**11.816**	**0**
1.6	3.489	0.055	12.172	0.384
2	3.823	0.222	14.570	1.698
2.5	4.498	0.364	20.097	3.272
3	4.521	1.800	17.197	16.272
3.5	3.676	2.042	9.347	15.013
4	3.822	1.862	11.140	14.232
4.5	4.183	2.890	9.143	24.178
5	2.422	4.049	−10.524	19.614
5.5	1.203	2.865	−6.762	6.896
6	1.331	2.140	−2.807	5.696
…				
10^{22}	**2.080**	**0**	**4.3266**	**0**
At x=0.5,				
E_{CPE} =1.6576	**3.269**	**0**	**10.689**	**0**
2	3.527	0.214	12.394	1.507
2.5	4.126	0.269	16.955	2.217
3	4.238	1.480	15.772	12.547
3.5	3.556	1.767	9.524	12.571
4	3.694	1.661	10.885	12.268
4.5	4.029	2.629	9.326	21.187
5	2.416	3.734	−8.109	18.042
5.5	1.270	2.670	−5.516	6.785
6	1.374	2.010	−2.152	5.524
…				
10^{22}	**1.9980**	**0**	**3.9922**	**0**
At x=1,				
E_{CPE} =1.7954	**3.098**	**0**	**9.598**	**0**
2	3.241	0.186	10.472	1.207
2.5	3.769	0.188	14.173	1.417
3	3.955	1.192	14.224	9.428
3.5	3.423	1.153	9.428	10.358
4	3.555	1.471	10.471	10.458
4.5	3.868	2.380	9.295	18.414
5	2.396	3.433	−6.045	16.447
5.5	1.323	2.482	−4.412	6.566
6	1.404	1.884	−1.580	5.292
…				
10^{22}	**1.9125**	**0**	**3.6577**	**0**
E in eV	n	κ	ε_1	ε_2

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

E in eV	n	κ	ε_1	ε_2
At x=0,				
E_{CPE} =1.5037	**4.173**	**0**	**17.414**	**0**
1.6	4.236	0.059	17.939	0.502
2	4.575	0.222	20.883	2.033
2.5	5.258	0.376	27.509	3.952
3	5.270	1.839	24.390	19.384
3.5	4.406	2.075	15.110	18.286
4	4.552	1.886	17.168	17.174
4.5	4.916	2.921	15.638	28.727
5	3.138	4.086	−6.847	25.649
5.5	1.911	2.888	−4.692	11.040
6	2.041	2.155	−0.477	8.799
...				
10^{22}	**2.8057**	**0**	**7.8719**	**0**
At x=0.5,				
E_{CPE} =1.6320	**3.9825**	**0**	**15.860**	**0**
2	4.263	0.216	18.125	1.845
2.5	4.876	0.285	23.693	2.782
3	4.972	1.537	22.362	15.288
3.5	4.261	1.817	14.856	15.485
4	4.400	1.697	16.477	14.936
4.5	4.740	2.677	15.305	25.376
5	3.099	3.792	−4.771	23.505
5.5	1.941	2.706	−3.557	10.503
6	2.048	2.034	0.059	8.333
...				
10^{22}	**2.6951**	**0**	**7.2634**	**0**
At x=1,				
E_{CPE} =1.7568	**3.7893**	**0**	**14.3590**	**0**
2	3.936	0.196	15.668	1.557
2.5	4.511	0.209	20.304	1.886
3	4.677	1.269	20.268	11.876
3.5	4.105	1.582	14.344	12.989
4	4.237	1.523	15.636	12.908
4.5	4.557	2.449	14.769	22.317
5	3.045	3.516	−3.087	21.416
5.5	1.952	2.534	−2.610	9.896
6	2.040	1.919	0.477	7.830
...				
10^{22}	**2.5797**	**0**	**6.6548**	**0**
E in eV	n	κ	ε_1	ε_2

Table 4n: In the X(x)-system, at E=3.2 eV and T=20 K, for given r_d and x, and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of $\eta_n(\gg 1$, degenerate case), E_{gn1}, n, κ, ε_1 and ε_2, obtained as functions of N, being represented by the arrows: ↗ and ↘, noting that both η_n and E_{gn1} increase with increasing N.

N (10^{18} cm^{-3})	↗	15	26	60	100
x=0					
For $\mathbf{r_d} = \mathbf{r_{As}}$,					
$\eta_n \gg 1$	↗	238	345	602	847
E_{gn1} in eV	↗	1.475	1.525	1.686	1.870
n	↘	4.247	4.201	4.046	3.865
κ	↘	2.206	2.080	1.698	1.311
ε_1	↗	13.175	13.319	13.489 ↘	13.221
ε_2	↘	18.736	17.473	13.744	10.137
For $\mathbf{r_d} = \mathbf{r_{Te}}$,					
$\eta_n \gg 1$	↗	239	345	602	847
E_{gn1} in eV	↗	1.497	1.554	1.731	1.928
n	↘	4.163	4.109	3.939	3.743
κ	↘	2.149	2.008	1.600	1.200
ε_1	↗	12.708	12.853	12.957 ↘	12.571
ε_2	↘	17.892	16.500	12.602	8.983
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↗	239	345	602	847
E_{gn1} in eV	↗	1.525	1.591	1.786	1.999
n	↘	4.054	3.992	3.802	3.587
κ	↘	2.080	1.920	1.481	1.068
ε_1		12.109 ↗	12.249 ↘	12.260	11.727
ε_2	↘	16.864	15.327	11.261	7.664
x=0.5					
For $\mathbf{r_d} = \mathbf{r_{As}}$,					
$\eta_n \gg 1$	↗	130	188	329	463
E_{gn1} in eV	↗	1.649	1.682	1.784	1.896
n	↘	4.001	3.969	3.870	3.758
κ	↘	1.783	1.707	1.487	1.261
ε_1		12.831 ↗	12.839 ↘	12.766	12.534
ε_2	↘	14.272	13.555	11.507	9.480
For $\mathbf{r_d} = \mathbf{r_{Te}}$,					
$\eta_n \gg 1$	↗	130	188	329	463
E_{gn1} in eV	↗	1.660	1.697	1.806	1.924
n	↘	3.929	3.893	3.786	3.668
κ	↘	1.757	1.674	1.440	1.206
ε_1		12.349 ↗	12.355 ↘	12.262	11.997
ε_2	↘	13.805	13.034	10.903	8.846
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↗	130	188	329	463
E_{gn1} in eV	↗	1.675	1.716	1.834	1.961
n	↘	3.835	3.795	3.679	3.551
κ	↘	1.724	1.632	1.382	1.138
ε_1		11.739 ↗	11.742 ↘	11.623	11.317
ε_2	↘	13.221	12.389	10.169	8.087
x=1					

For $\mathbf{r_d} = \mathbf{r_{As}}$,					
$\eta_n \gg 1$	↗	93	135	236	331
E_{gn1} in eV	↗	1.815	1.847	1.938	2.034
n	↘	3.754	3.722	3.630	3.532
κ	↘	1.422	1.356	1.180	1.008
ε_1	↘	12.073	12.015	11.788	11.462
ε_2	↘	10.679	10.098	8.568	7.120
For $\mathbf{r_d} = \mathbf{r_{Te}}$,					
$\eta_n \gg 1$	↗	93	134.5	236	331
E_{gn1} in eV	↗	1.822	1.857	1.952	2.051
n	↘	3.688	3.654	3.557	3.455
κ	↘	1.406	1.337	1.154	0.978
ε_1	↘	11.623	11.562	11.324	10.984
ε_2	↘	10.375	9.772	8.212	6.757
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↗	93	134.3	235	331
E_{gn1} in eV	↗	1.832	1.869	1.970	2.074
n	↘	3.602	3.565	3.463	3.356
κ	↘	1.386	1.312	1.122	0.940
ε_1	↘	11.054	10.989	10.738	10.381
ε_2	↘	9.988	9.361	7.770	6.311
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 η_p($\gg$ 1, degenerate case), E_{gp1}, n, κ, ε_1 and ε_2, obtained as functions of N, being represented by the arrows: ↗ and ↘, noting that both η_p and E_{gp1} increase with increasing N.

N (10^{18} cm^{-3})	↗	15	26	60	100
			x=0		
For $\mathbf{r_a} = \mathbf{r_{Ga}}$,					
$\eta_p \gg 1$	↗	227	335	595	840
E_{gp1} in eV	↗	1.869	2.043	2.466	2.869
n	↘	3.866	3.690	3.234	2.772
κ	↘	1.313	0.992	0.399	0.081
ε_1	↘	13.223	12.623	10.303	7.676
ε_2	↘	10.156	7.320	2.581	0.450
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↗	223	332	592	838
E_{gp1} in eV	↗	1.869	2.045	2.472	2.876
n	↘	3.775	3.596	3.138	2.672
κ	↘	1.312	0.988	0.393	0.077
ε_1	↘	12.529	11.953	9.692	7.135
ε_2	↘	9.909	7.106	2.468	0.415

For $\mathbf{r_a} = \mathbf{r_{Cd}}$,					
$\eta_p \gg 1$	$\nearrow$	221	330	592	837
E_{gp1} in eV	$\nearrow$	1.869	2.046	2.474	2.880
n	$\searrow$	3.735	3.555	3.095	2.628
κ	$\searrow$	1.313	0.987	0.391	0.076
ε_1	$\searrow$	12.230	11.664	9.430	6.904
ε_2	$\searrow$	9.808	7.016	2.420	0.400
			x=0.5		
For $\mathbf{r_a} = \mathbf{r_{Ga}}$,					
$\eta_p \gg 1$	$\nearrow$	108	171	316	452
E_{gp1} in eV	$\nearrow$	1.820	1.919	2.155	2.377
n	$\searrow$	3.834	3.734	3.491	3.252
κ	$\searrow$	1.411	1.215	0.809	0.502
ε_1	$\searrow$	12.706	12.467	11.529	10.323
ε_2	$\searrow$	10.818	9.077	5.651	3.266
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	$\nearrow$	101	165	312	448
E_{gp1} in eV	$\nearrow$	1.817	1.919	2.158	2.3827
n	$\searrow$	3.750	3.648	3.401	3.160
κ	$\searrow$	1.418	1.216	0.805	0.496
ε_1	$\searrow$	12.052	11.825	10.916	9.737
ε_2	$\searrow$	10.635	8.875	5.476	3.137
For $\mathbf{r_a} = \mathbf{r_{Cd}}$,					
$\eta_p \gg 1$	$\nearrow$	97	161	309	446
E_{gp1} in eV	$\nearrow$	1.814	1.918	2.159	2.384
n	$\searrow$	3.714	3.610	3.361	3.119
κ	$\searrow$	1.423	1.218	0.804	0.494
ε_1	$\searrow$	12.989	11.550	10.652	9.485
ε_2	$\searrow$	11.769	8.796	5.403	3.082
			x=1		
For $\mathbf{r_a} = \mathbf{r_{Ga}}$,					
$\eta_p \gg 1$	$\nearrow$	47	99	210	310
E_{gp1} in eV	$\nearrow$	1.864	1.947	2.127	2.291
n	$\searrow$	3.706	3.622	3.436	3.261
κ	$\searrow$	1.324	1.164	0.854	0.612
ε_1	$\searrow$	11.980	11.762	11.075	10.257
ε_2	$\searrow$	9.810	8.432	5.866	3.993
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	$\nearrow$	28	87	202	303
E_{gp1} in eV	$\nearrow$	1.844	1.938	2.125	2.293
n	$\searrow$	3.642	3.547	3.354	3.176
κ	$\searrow$	1.363	1.180	0.856	0.610
ε_1	$\searrow$	11.406	11.189	10.515	9.712
ε_2	$\searrow$	9.925	8.369	5.741	3.876
For $\mathbf{r_a} = \mathbf{r_{Cd}}$,					
$\eta_p \gg 1$	$\nearrow$	13	80	197	300
E_{gp1} in eV	$\nearrow$	1.827	1.933	2.124	2.293
n	$\searrow$	3.622	3.516	3.319	3.139
κ	$\searrow$	1.397	1.191	0.858	0.610
ε_1	$\searrow$	11.168	10.946	10.277	9.480
ε_2	$\searrow$	10.119	8.373	5.697	3.830
N (10^{18} cm^{-3})	$\nearrow$	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 $\mathbf{r_d} = \mathbf{r_{As}}$,						
$\eta_n \gg 1$	↘	847	339	169	56	
E_{gn1} in eV	↘	1.870	1.866	1.853	1.774	
n	↗	3.865	3.870		3.882	3.961
κ	↗	1.311	1.320	1.345	1.507	
ε_1	↗	13.221	13.232	13.263	13.415	
ε_2	↗	10.132	10.215	10.441	11.940	
For $\mathbf{r_d} = \mathbf{r_{Te}}$,						
$\eta_n \gg 1$	↘	847	339	169	56	
E_{gn1} in eV	↘	1.928	1.923	1.911	1.832	
n	↗	3.743	3.747	3.760	3.839	
κ	↗	1.200	1.208	1.232	1.388	
ε_1	↗	12.571	12.584	12.621	12.816	
ε_2	↗	8.983	9.055	9.264	10.656	
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,						
$\eta_n \gg 1$	↘	847	339	169	56	
E_{gn1} in eV	↘	1.999	1.995	1.983	1.904	
n	↗	3.587	3.592	3.604	3.685	
κ	↗	1.068	1.076	1.098	1.246	
ε_1	↗	11.727	11.742	11.785	12.026	
ε_2	↗	7.664	7.729	7.919	9.181	
			x=0.5			
For $\mathbf{r_d} = \mathbf{r_{As}}$,						
$\eta_n \gg 1$	↘	463	185	93	31	
E_{gn1} in eV	↘	1.896	1.888	1.870	1.766	
n	↗	3.758	3.765	3.784	3.887	
κ	↗	1.261	1.275	1.311	1.524	
ε_1	↗	12.534	12.553	12.600	12.788	
ε_2	↗	9.480	9.603	9.926	11.849	
For $\mathbf{r_d} = \mathbf{r_{Te}}$,						
$\eta_n \gg 1$	↘	463	185	93	31	
E_{gn1} in eV	↘	1.924	1.917	1.899	1.795	
n	↗	3.668	3.675	3.694	3.797	
κ	↗	1.206	1.219	1.255	1.463	
ε_1	↗	11.997	12.018	12.068	12.279	
ε_2	↗	8.846	8.963	9.273	11.113	

For $\mathbf{r_d} = \mathbf{r_{Sn}}$,

$\eta_n \gg 1$	↘	463	185	92.6	31.8
E_{gn1} in eV	↘	1.961	1.953	1.935	1.831
n	↗	3.551	3.559	3.578	3.682
κ	↗	1.138	1.152	1.186	1.389
ε_1	↗	11.317	11.339	11.393	11.629
ε_2	↗	8.087	8.198	8.489	10.228

x=1

For $\mathbf{r_d} = \mathbf{r_{As}}$,

$\eta_n \gg 1$	↘	331.6	133.6	66	22
E_{gn1} in eV	↘	2.034	2.024	1.999	1.871
n	↗	3.532	3.543	3.568	3.698
κ	↗	1.008	1.025	1.069	1.309
ε_1	↗	11.462	11.500	11.590	11.964
ε_2	↗	7.120	7.264	7.627	9.685

For $\mathbf{r_d} = \mathbf{r_{Te}}$,

$\eta_n \gg 1$	↘	331.5	132.6	66	22
E_{gn1} in eV	↘	2.051	2.041	2.017	1.888
n	↗	3.455	3.466	3.491	3.622
κ	↗	0.978	0.995	1.038	1.275
ε_1	↗	10.984	11.022	11.113	11.493
ε_2	↗	6.757	6.896	7.246	9.236

For $\mathbf{r_d} = \mathbf{r_{Sn}}$,

$\eta_n \gg 1$	↘	331.4	132.5	66	22
E_{gn1} in eV	↘	2.074	2.064	2.039	1.911
n	↗	3.356	3.367	3.392	3.523
κ	↗	0.940	0.957	0.999	1.232

Table 5p. In the X(x)-system, at E=3.2 eV and $N = 10^{20} cm^{-3}$, for given r_a and x, and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of $\eta_p (\gg 1,$ degenerate case$)$, E_{gp1}, n, κ, ε_1 and ε_2, obtained as functions of T, being represented by the arrows: ↗ and ↘, noting that both η_p and E_{gp1} decrease with increasing T.

T in K	↗	20	50	100	300	
			x=0			
For $\mathbf{r_a} = \mathbf{r_{Ga}}$,						
$\eta_p \gg 1$	↘	840	336	168	56	
E_{gp1} in eV	↘	2.869	2.865	2.852	2.773	
n	↗	2.772	2.777		2.792	2.885
κ	↗	0.081	0.083	0.090	0.135	
ε_1	↗	7.676	7.704	7.785	8.303	
ε_2	↗	0.450	0.463	0.501	0.779	
For $\mathbf{r_a} = \mathbf{r_{In}}$,						
$\eta_p \gg 1$	↘	838	335	168	56	
E_{gp1} in eV	↘	2.876	2.872	2.860	2.780	
n	↗	2.672	2.677		2.692	2.785
κ	↗	0.077	0.080	0.086	0.130	
ε_1	↗	7.135	7.162	7.241	7.741	
ε_2	↗	0.415	0.427	0.462	0.726	
For $\mathbf{r_a} = \mathbf{r_{Cd}}$,						
$\eta_p \gg 1$	↘	837	335	167	56	
E_{gp1} in eV	↘	2.880	2.875	2.863	2.784	
n	↗	2.628	2.634		2.648	2.742
κ	↗	0.076	0.078	0.084	0.128	
ε_1	↗	6.904	6.931	7.008	7.500	
ε_2	↗	0.400	0.412	0.446	0.704	
			x=0.5			
For $\mathbf{r_a} = \mathbf{r_{Ga}}$,						
$\eta_p \gg 1$	↘	452	181	90	30	
E_{gp1} in eV	↘	2.377	2.370	2.351	2.247	
n	↗	3.252	3.260	3.280	3.392	
κ	↗	0.502	0.511	0.534	0.673	
ε_1	↗	10.323	10.365	10.474	11.056	
ε_2	↗	3.266	3.331	3.504	4.563	
For $\mathbf{r_a} = \mathbf{r_{In}}$,						
$\eta_p \gg 1$	↘	448	179	89.7	29.9	
E_{gp1} in eV	↘	2.382	2.374	2.356	2.252	
n	↗	3.160	3.167	3.188	3.300	
κ	↗	0.496	0.505	0.528	0.666	
ε_1	↗	9.737	9.778	9.884	10.448	
ε_2	↗	3.137	3.200	3.367	4.395	
For $\mathbf{r_a} = \mathbf{r_{Cd}}$,						

$\eta_p \gg 1$	↘	446	178	89.3	29.7
E_{gp1} in eV	↘	2.384	2.376	2.358	2.254
n	↗	3.119	3.127	3.147	3.260
κ	↗	0.494	0.503	0.526	0.663
ε_1	↗	9.485	9.526	9.630	10.186
ε_2	↗	3.082	3.145	3.310	4.324
			x=1		
For $\mathbf{r_a} = \mathbf{r_{Ga}}$,					
$\eta_p \gg 1$	↘	310	124	62	20.6
E_{gp1} in eV	↘	2.291	2.281	2.256	2.128
n	↗	3.261	3.271	3.298	3.434
κ	↗	0.612	0.626	0.660	0.852
ε_1	↗	10.257	10.311	10.442	11.070
ε_2	↗	3.993	4.095	4.353	5.851
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↘	303	121	61	20.2
E_{gp1} in eV	↘	2.293	2.283	2.258	2.129
n	↗	3.176	3.186	3.213	3.349
κ	↗	0.610	0.624	0.658	0.849
ε_1	↗	9.712	9.764	9.891	10.497
ε_2	↗	3.876	3.976	4.228	5.690
For $\mathbf{r_a} = \mathbf{r_{Cd}}$,					
$\eta_p \gg 1$	↘	300	120	60	20
E_{gp1} in eV	↘	2.292	2.283	2.258	2.130
n	↗	3.139	3.150	3.176	3.313
κ	↗	0.610	0.624	0.658	0.849
ε_1	↗	9.480	9.531	9.656	10.253
ε_2	↗	3.830	3.928	4.178	5.626
T in K	↗	20	50	100	300