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

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ABTRACT

In the n(p)-type $GaAs_{1-x}Te_x$- 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 2.89×10^{-7} the density of carriers localized in exponential band tails, with a precision of the order of, 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 $\varepsilon(r_{d(a)}, x)$ $N^*(N, r_{d(a)}, x)$ -law and to the effective density of electrons (holes) given in parabolic conduction (valence) bands, 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: $GaAs_{1-x}Te_x$- 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 $X(x) \equiv GaAs_{1-x}Te_x$- 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: $r_{do(ao)}$=$r_{As(Ga)}$=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: $m_{c(v)}(x)/m_o = 0.209(0.4) \times x + 0.066\ (0.291) \times (1-x)$ (1)

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

$$\varepsilon_o(x) = 12.3 \times x + 13.13 \times (1-x). \qquad (2)$$

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

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

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:

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

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:

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

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

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

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**,

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

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 $N = N_{CDn(CDp)}(r_{d(a)}, x)$: $r_{sn(sp)}(N_{CDn(CDp)}(r_{d(a)}, x), r_{d(a)}, x) =$ **2.4814**, 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 $\mathcal{H}_{n(p)} = \mathbf{0.47137}$, 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 $\mathbf{2.89 \times 10^{-7}}$. 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:

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

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

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

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

where $m_r(x)/m_c$ 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:

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

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:

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

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

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

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

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

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

One also remarks that, as $N^* = 0$, according to the MIT, $\Delta E_{gn(gp)}(N, r_{d(a)}, x) = 0$.

OPTICAL BAND GAP

Here, the optical band gap is found to be defined by:

$$E_{gn1(gp1)}(N, r_{d(a)}, x, T) \equiv E_{gni(gpi)}(r_{d(a)}, x, T) - \Delta E_{gn(gp)}(N, r_{d(a)}, x) + (-)E_{Fn(Fp)}(N, r_{d(a)}, x, T) \quad (15)$$

where $E_{gin(gip)}$, $[+E_{Fn}, -E_{Fp}] \geq 0$, and $\Delta E_{gn(gp)}$ are respectively determined in Equations [10, 12, 14n(p)], respectively. So, as noted above, at the MIT, Eq. (15) thus becomes: $E_{gn1(gp1)}(r_{d(a)}, x) = E_{gno(gpo)}(r_{d(a)}, x)$, according to: $N = N_{CDn(NDp)}(r_{d(a)}, x)$.

OPTICAL COEFFICIENTS

The optical properties of any medium can be described by the complex refraction index $\mathbb{N}$ and the complex dielectric function ε, $\mathbb{N} \equiv n - i\kappa$ and $\varepsilon \equiv \varepsilon_1 - i\varepsilon_2$, where $i^2 = -1$ and $\varepsilon \equiv \mathbb{N}^2$. Therefore, the real and imaginary parts of ε denoted by ε_1 and ε_2 can thus be expressed in terms of the refraction index n and the extinction coefficient κ as: $\varepsilon_1 \equiv n^2 - \kappa^2$ and $\varepsilon_2 \equiv 2n\kappa$. One notes that the optical absorption coefficient α is related to ε_2, n, κ, and the optical conductivity σ_O, by[2]

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

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

Here, -q, $\hbar$, $|v(E)|$, ω, $\varepsilon_{free\,space}$, c and $J(E^*)$ respectively represent: the electron charge, Dirac's constant, matrix elements of the velocity operator between valence (conduction)-and-conduction (valence) bands in n(p)-type semiconductors, photon frequency, permittivity of free space, velocity of light, and joint density of states. It should be noted that, if the three functions such as: $|v(E)|^2$, $J(E^*)$ and $n(E)$ are known, then the other optical dispersion functions as those given in Eq. (16) can thus be determined. Moreover, the normal- incidence reflectance, $R(E)$, can be expressed in terms of $\kappa(E)$ and $n(E)$ as:

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

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

Then, one has:

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

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

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

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

Further, one notes that, as $E \to \infty$, Forouhi and Bloomer (FB) [4] claimed that $\kappa(E \to \infty) \to$ a constant, while the $\kappa(E)$ -expressions, proposed by Van Cong [2] quickly go to 0 as E^{-3}, and consequently, their numerical results of the optical functions such as: $\sigma_O(E)$ and $\alpha(E)$, given in Eq. (16), both go to 0 as E^{-2}.

Now, an improved Forouhi-Bloomer parameterization model (FB-PM), used to determine the expressions of the optical coefficients in the degenerate $n^+(p^+) - p(n)\, X(x)$- crystalline alloy, is now proposed as follows. Then, if denoting the functions G(E) and F(E) and by: $G(E) \equiv \sum_{i=1}^{4} \frac{A_i}{E^2 - B_i E + C_i}$ and $F(E) \equiv \sum_{i=1}^{4} \frac{A_i}{E^2 \times (1 + 10^{-4} \times \frac{E}{6}) - B_i E + C_i}$, we propose:

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

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

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,

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

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 following cases.

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 $E \to \infty$

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 $R_{\infty}(r_{d(a)}, x)$ 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 $\eta_{n(p)}(\gg 1, \text{degenerate case})$, $E_{gn1(gp1)}$, 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 $GaAs_{1-x}Te_x$- 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 2.89×10^{-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	↗	1657.5	1658	1659.5	1660.6	1662
n_{MIT}	↘	3.318	3.297	3.233	3.195	3.151
$\varepsilon_{1(MIT)}$	↘	11.01	10.87	10.45	10.21	9.93
R_{MIT}	↘	0.288	0.286	0.278	0.274	0.268
At x=1,						
E_{CPE} in meV	↗	1795.2	1796	1798.5	1800.2	1802.4
n_{MIT}	↘	3.199	3.178	3.114	3.076	3.032
$\varepsilon_{1(MIT)}$	↘	10.23	10.10	9.70	9.46	9.19
R_{MIT}	↘	0.274	0.272	0.264	0.259	0.254

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	↗	1637	1658	1661	1664	1667
n_{MIT}	↘	4.045	3.297	3.240	3.204	3.163
$\varepsilon_{1(MIT)}$	↘	16.36	10.87	10.496	10.27	10.01
R_{MIT}	↘	0.364	0.286	0.279	0.275	0.270

At x=1,						
E_{CPE} in meV	↗	1770	1796	1800	1803	1807
n_{MIT}	↘	3.917	3.178	3.121	3.086	3.045
$\varepsilon_{1(MIT)}$	↘	15.34	10.10	9.739	9.52	9.271
R_{MIT}	↘	0.352	0.272	0.265	0.261	0.250

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	1.9952	1.9568	1.9126
$\varepsilon_{1,\infty}$	↘	4.327	4.2392	3.9809	3.8292	3.6581
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	9.4912	9.3951	9.1044	8.9292	8.7274
α_∞ in $(10^5 \times cm^{-1})$		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_∞	↘	2.047	2.026	1.963	1.925	1.882
$\varepsilon_{1,\infty}$	↘	4.190	4.105	3.854	3.707	3.541
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	9.340	9.245	8.958	8.786	8.587
α_∞ in $(10^5 \times cm^{-1})$		2.160	2.160	2.160	2.160	2.160
R_∞	↘	0.118	0.115	0.106	0.100	0.094
At x=1,						
n_∞	↘	2.013	1.993	1.931	1.894	1.851
$\varepsilon_{1,\infty}$	↘	4.053	3.971	3.728	3.586	3.426
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	9.186	9.093	8.811	8.641	8.446
α_∞ in $(10^5 \times cm^{-1})$		2.160	2.160	2.160	2.160	2.160
R_∞	↘	0.113	0.110	0.101	0.095	0.089

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 $(10^5 \times cm^{-1})$		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_∞	↘	2.761	2.026	1.971	1.937	1.898
$\varepsilon_{1,\infty}$	↘	7.623	4.105	3.883	3.752	3.601
$\sigma_{O,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	12.60	9.245	8.992	8.838	8.659
α_∞ in $(10^7 \times cm^{-1})$	2.160	2.160	2.160	2.160	2.160	
R_∞	↘	0.219	0.115	0.107	0.102	0.096
At x=1,						
n_∞	↘	2.715	1.993	1.938	1.905	1.866
$\varepsilon_{1,\infty}$	↘	7.374	3.971	3.757	3.629	3.483
$\sigma_{O,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	12.39	9.093	8.844	8.693	8.517
α_∞ in $(10^7 \times cm^{-1})$		2.160	2.160	2.160	2.160	2.160
R_∞	↘	0.213	0.110	0.102	0.097	0.091

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) $\kappa = 0$

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	0.508
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	15.010
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}	**2.08**	**0**	**4.326**	**0**

At x=0.5,				
E_{CPE} =1.6575	**3.318**	**0**	**11.012**	**0**
2	3.576	0.214	12.742	1.528
2.5	4.175	0.269	17.362	2.244
3	4.287	1.480	16.190	12.694
3.5	3.605	1.768	9.873	12.746
4	3.742	1.661	11.248	12.432
4.5	4.078	2.629	9.721	21.446
5	2.464	3.734	−7.823	18.408
5.5	1.319	2.670	−5.391	7.046
6	1.423	2.010	−2.016	5.720
…				
10^{22}	**2.047**	**0**	**4.190**	**0**
At x=1,				
E_{CPE} =1.7952	**3.199**	**0**	**10.233**	**0**
2	3.342	0.186	11.136	1.245
2.5	3.870	0.188	14.945	1.455
3	4.056	1.192	15.032	9.672
3.5	3.524	1.513	10.128	10.665
4	3.655	1.471	11.197	10.757
4.5	3.969	2.381	10.084	18.896
5	2.496	3.433	−5.555	17.140
5.5	1.423	2.482	−4.137	7.066
6	1.505	1.885	−1.288	5.672
…				
10^{22}	**2.013**	**0**	**4.053**	**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} =1.6374	**4.045**	**0**	**16.362**	**0**
2	4.321	0.216	18.621	1.865
2.5	4.931	0.282	24.233	2.778
3	5.030	1.525	22.980	15.345
3.5	4.325	1.806	15.446	15.629
4	4.464	1.690	17.071	15.084
4.5	4.803	2.667	15.961	25.617
5	3.168	3.780	−4.249	23.950
5.5	2.012	2.698	−3.233	10.860
6	2.119	2.029	0.374	8.599

…				
10^{22}	**2.761**	**0**	**7.6231**	**0**
At x=1,				
E_{CPE} =1.7705	**3.9167**	**0**	**15.3404**	**0**
2	4.079	0.193	16.606	1.575
2.5	4.620	0.201	21.306	1.862
3	4.794	1.242	21.439	11.906
3.5	4.235	1.557	15.513	13.194
4	4.369	1.505	16.814	13.144
4.5	4.685	2.424	16.073	22.117
5	3.187	3.486	−1.995	22.226
5.5	2.102	2.516	−1.912	10.575
6	2.187	1.907	1.146	8.341
…				
10^{22}	**2.7156**	**0**	**7.3743**	**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 $r_d = r_{As}$,						
$\eta_n \gg 1$	↗	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 $r_d = r_{Te}$,						
$\eta_n \gg 1$	↗	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	↗	1.724	1.780	1.930	2.082
n	↘	3.977	3.922	3.772	3.616
κ	↘	1.614	1.495	1.196	0.927
ε_1	↘	13.208	13.148	12.799	12.215
ε_2	↘	12.842	11.724	9.027	6.701
For $\mathbf{r_d} = \mathbf{r_{Te}}$,					
$\eta_n \gg 1$	↗	130	188	329	463
E_{gn1} in eV	↗	1.732	1.790	1.945	2.101
n	↘	3.906	3.849	3.694	3.533
κ	↘	1.597	1.473	1.168	0.895
ε_1	↘	12.707	12.644	12.282	11.679
ε_2	↘	12.478	11.342	8.632	6.325
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↗	129	188	329	463
E_{gn1} in eV	↗	1.742	1.803	1.964	2.125

n	↘	3.815	3.755	3.593	3.426
κ	↘	1.575	1.446	1.133	0.856
ε_1	↘	12.072	12.007	11.629	11.005
ε_2	↘	12.017	10.861	8.144	5.868
			x=1		
For $r_d = r_{As}$,					
$\eta_n \gg 1$	↗	91	133	235	331
E_{gn1} in eV	↗	1.802	1.831	1.914	2.003
n	↘	3.900	3.871	3.788	3.698
κ	↘	1.448	1.389	1.226	1.063
ε_1	↘	13.112	13.058	12.847	12.544
ε_2	↘	11.291	10.756	9.290	7.860
For $r_d = r_{Te}$,					
$\eta_n \gg 1$	↗	91	133	234	330
E_{gn1} in eV	↗	1.811	1.842	1.930	2.023
n	↘	3.828	3.797	3.709	3.614
κ	↘	1.429	1.367	1.196	1.028
ε_1	↘	12.610	12.552	12.328	12.007
ε_2	↘	10.941	10.379	8.873	7.429
For $r_d = r_{Sn}$,					
$\eta_n \gg 1$	↗	90	132	234	330
E_{gn1} in eV	↗	1.823	1.857	1.950	2.048
n	↘	3.735	3.701	3.607	3.507
κ	↘	1.405	1.337	1.158	0.984
ε_1	↘	11.975	11.912	11.671	11.329
ε_2	↘	10.495	9.902	8.353	6.900
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 $\eta_p (\gg 1$, 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 $r_a = r_{Ga}$,				
$\eta_p \gg 1$ ↗	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 $r_a = r_{In}$,				
$\eta_p \gg 1$ ↗	223	332	592	838
E_{gp1} in eV ↗	1.860	2.036	2.463	2.867
n ↘	3.784	3.605	3.148	2.683
κ ↘	1.330	1.004	0.403	0.082
ε_1 ↘	12.551	11.989	9.747	7.192
ε_2 ↘	10.068	7.236	2.538	0.440
For $r_a = r_{Cd}$,				
$\eta_p \gg 1$ ↗	221	330	592	837
E_{gp1} in eV ↗	1.855	2.032	2.460	2.866
n ↘	3.749	3.569	3.111	2.645
κ ↘	1.340	1.010	0.406	0.083
ε_1 ↘	12.261	11.719	9.513	6.989
ε_2 ↘	10.049	7.213	2.525	0.438
x=0.5				
For $r_a = r_{Ga}$,				
$\eta_p \gg 1$ ↗	118	178	322	457
E_{gp1} in eV ↗	1.829	1.923	2.152	2.368
n ↘	3.873	3.778	3.543	3.310
κ ↘	1.393	1.208	0.815	0.512
ε_1 ↘	13.062	12.818	11.887	10.691
ε_2 ↘	10.789	9.128	5.773	3.393
For $r_a = r_{In}$,				
$\eta_p \gg 1$ ↗	114	175	319	455
E_{gp1} in eV ↗	1.819	1.915	2.145	2.364
n ↘	3.794	3.698	3.460	3.225
κ ↘	1.414	1.224	0.824	0.518
ε_1 ↘	12.397	12.177	11.292	10.134
ε_2 ↘	10.732	9.057	5.706	3.343

For $\mathbf{r_a} = \mathbf{r_{Cd}}$,					
$\eta_p \gg 1$	↗	112	173	318	454
E_{gp1} in eV	↗	1.813	1.910	2.142	2.361
n	↘	3.761	3.664	3.425	3.189
κ	↘	1.426	1.234	0.830	0.522
ε_1	↘	12.111	11.901	11.039	9.899
ε_2	↘	10.729	9.043	5.687	3.328
			x=1		
For $\mathbf{r_a} = \mathbf{r_{Ga}}$,					
$\eta_p \gg 1$	↗	78	122	226	324
E_{gp1} in eV	↗	1.904	1.973	2.137	2.293
n	↘	3.764	3.694	3.524	3.358
κ	↘	1.244	1.115	0.837	0.610
ε_1	↘	12.623	12.405	11.720	10.907
ε_2	↘	9.367	8.243	5.899	4.097
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↗	73	118	223	321
E_{gp1} in eV	↗	1.890	1.961	2.128	2.285
n	↘	3.691	3.619	3.446	3.279
κ	↘	1.271	1.137	0.852	0.620
ε_1	↘	12.006	11.804	11.152	10.368
ε_2	↘	9.384	8.234	5.871	4.070
For $\mathbf{r_a} = \mathbf{r_{Cd}}$,					
$\eta_p \gg 1$	↗	70	116	222	320
E_{gp1} in eV	↗	1.883	1.954	2.123	2.280
n	↘	3.660	3.587	3.414	3.245
κ	↘	1.286	1.150	0.860	0.627
ε_1	↘	11.741	11.546	10.910	10.140
ε_2	↘	9.417	8.249	5.872	4.068
N (10^{18} cm^{-3})	↗	15	26	60	100

Table 5n: In the X(x)-system, at E=3.2 eV and $N = 10^{20} cm^{-3}$, for given r_d and x, and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of $\eta_n (\gg 1$, degenerate case), E_{gn1}, n, κ, ε_1 and ε_2, obtained as functions of T, being represented by the arrows: ↗ and ↘, noting that both η_n and E_{gn1} decrease with increasing T.

T in K	↗	20	50	100	300	
			x=0			
For $\mathbf{r_d} = \mathbf{r_{As}}$,						
$\eta_n \gg 1$	↘	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	92	31	
E_{gn1} in eV	↘	2.083	2.075	2.056	1.952	
n	↗	3.615	3.623	3.642	3.749	
κ	↗	0.925	0.939	0.970	1.154	
ε_1	↗	12.211	12.246	12.327	12.725	
ε_2	↗	6.691	6.801	7.066	8.651	
For $\mathbf{r_d} = \mathbf{r_{Te}}$,						
$\eta_n \gg 1$	↘	463	185	92	31	
E_{gn1} in eV	↘	2.101	2.094	2.075	1.971	

n	↗	3.533	3.540	3.560	3.700
κ	↗	0.895	0.907	0.938	1.118
ε_1	↗	11.679	11.711	11.792	12.193
ε_2	↗	6.325	6.421	6.676	8.203
For $r_d = r_{Sn}$,					
$\eta_n \gg 1$	↘	463	185	92	31
E_{gn1} in eV	↘	2.125	2.118	2.099	1.996
n	↗	3.426	3.434	3.453	3.561
κ	↗	0.856	0.868	0.898	1.075
ε_1	↗	11.005	11.037	11.118	11.522
ε_2	↗	5.868	5.959	6.201	7.656
			x=1		
For $r_d = r_{As}$,					
$\eta_n \gg 1$	↘	331	132	66	22
E_{gn1} in eV	↘	2.166	2.156	2.131	2.003
n	↗	3.494	3.505	3.531	3.664
κ	↗	0.793	0.808	0.847	1.062
ε_1	↗	11.582	11.631	11.750	12.298
ε_2	↗	5.541	5.666	5.981	7.786
For $r_d = r_{Te}$,					
$\eta_n \gg 1$	↘	330	132	66	22
E_{gn1} in eV	↘	2.177	2.167	2.142	2.014
n	↗	3.421	3.431	3.457	3.591
κ	↗	0.776	0.791	0.830	1.043
ε_1	↗	11.099	11.148	11.266	11.808
ε_2	↗	5.309	5.430	5.737	7.491
For $r_d = r_{Sn}$,					
$\eta_n \gg 1$	↘	330	132	66	22
E_{gn1} in eV	↘	2.191	2.181	2.156	2.028
n	↗	3.326	3.336	3.362	3.496
κ	↗	0.755	0.770	0.807	1.018
ε_1	↗	10.491	10.539	10.654	11.188
ε_2	↗	5.019	5.136	5.430	7.120
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 $r_a = r_{Ga}$,						
$\eta_p \gg 1$	↘	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 $r_a = r_{In}$,						
$\eta_p \gg 1$	↘	838	335	168	56	
E_{gp1} in eV	↘	2.867	2.863	2.850	2.771	
n	↗	2.683	2.688		2.703	2.796
κ	↗	0.082	0.084	0.090	0.136	
ε_1	↗	7.192	7.219	7.298	7.798	
ε_2	↗	0.440	0.452	0.489	0.761	
For $r_a = r_{Cd}$,						
$\eta_p \gg 1$	↘	837	335	167	56	
E_{gp1} in eV	↘	2.866	2.861	2.849	2.770	

n	↗	2.645	2.650		2.665	2.758
κ	↗	0.083	0.085	0.091	0.137	
ε_1	↗	6.990	7.016	7.093	7.586	
ε_2	↗	0.438	0.450	0.487	0.756	
		x=0.5				
For $r_a = r_{Ga}$,						
$\eta_p \gg 1$	↘	457	183	91	30	
E_{gp1} in eV	↘	2.368	2.361	2.343	2.239	
n	↗	3.310	3.317	3.338	3.450	
κ	↗	0.512	0.521	0.545	0.685	
ε_1	↗	10.691	10.734	10.844	11.432	
ε_2	↗	3.393	3.460	3.637	4.724	
For $r_a = r_{In}$,						
$\eta_p \gg 1$	↘	455	182	91	30	
E_{gp1} in eV	↘	2.364	2.357	2.338	2.234	
n	↗	3.225	3.233	3.353	3.365	
κ	↗	0.518	0.527	0.551	0.691	
ε_1	↗	10.134	10.176	10.282	10.849	
ε_2	↗	3.343	3.409	3.583	4.652	
For $r_a = r_{Cd}$,						
$\eta_p \gg 1$	↘	454	181	91	30	
E_{gp1} in eV	↘	2.361	2.354	2.335	2.231	
n	↗	3.189	3.197	3.217	3.329	
κ	↗	0.522	0.531	0.554	0.695	
ε_1	↗	9.899	9.940	10.044	10.601	
ε_2	↗	3.328	3.394	3.567	4.630	
		x=1				
For $r_a = r_{Ga}$,						
$\eta_p \gg 1$	↘	324	129	65	21	
E_{gp1} in eV	↘	2.293	2.283	2.258	2.130	
n	↗	3.358	3.369	3.396	3.532	
κ	↗	0.610	0.623	0.657	0.849	
ε_1	↗	10.907	10.963	11.100	11.756	
ε_2	↗	4.097	4.202	4.466	5.998	
For $r_a = r_{In}$,						
$\eta_p \gg 1$	↘	321	128	64	21	
E_{gp1} in eV	↘	2.285	2.275	2.250	2.122	

n	↗	3.279	3.290	3.316	3.453
κ	↗	0.620	0.634	0.668	0.861
ε_1	↗	10.368	10.422	10.522	11.179
ε_2	↗	4.070	4.173	4.434	5.948
For $r_a = r_{Cd}$,					
$\eta_p \gg 1$	↘	320	128	64	21
E_{gp1} in eV	↘	2.280	2.270	2.246	2.117
n	↗	3.245	3.256	3.283	3.419
κ	↗	0.627	0.640	0.675	0.869
ε_1	↗	10.140	10.193	10.321	10.934
ε_2	↗	4.068	4.171	4.431	5.940
T in K	↗	20	50	100	300