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OPTICAL COEFFICIENTS IN THE N(P)-TYPE DEGENERATE GaTe(1-x) P(x)-CRYSTALLINE ALLOY, DUE TO THE NEW STATIC DIELECTRIC CONSTANT-LAW AND THE GENERALIZED MOTT CRITERIUM IN THE METAL-INSULATOR TRANSITION (8)

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ABTRACT

In the n(p)-type $GaTe_{1-x}P_x$- 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 2.91×10^{-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: $GaTe_{1-x}P_x$- crystalline alloy; impurity-size effect; Mott critical impurity density in the MIT, optical coefficients.

INTRODUCTION

Here, basing on our two recent works[1, 2] and also other ones[3-8], all the optical coefficients given in the n(p)-type $\mathbf{X(x) \equiv GaTe_{1-x}P_x}$ - 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: $r_{do(ao)} = r_{Te(Ga)}$=0.132 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:

$$m_{c(v)}(x)/m_o = 0.13\ (0.5) \times x + 0.209\ (0.4) \times (1-x) \quad (1)$$

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

$$\varepsilon_o(x) = 11.1 \times x + 12.3 \times (1-x). \quad (2)$$

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

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

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 $V = (4\pi/3)\times\left(r_{d(a)}\right)^3$, $V_{do(ao)} = (4\pi/3)\times\left(r_{do(ao)}\right)^3$, for the pressure p, $p_o = 0$, and for the deformation potential energy (or the strain energy) σ, $\sigma_o = 0$. Further, the two important equations[1, 7], used to determine the σ-variation, $\Delta\sigma \equiv \sigma - \sigma_o = \sigma$, are defined by: $\frac{dp}{dV} = -\frac{B}{V}$ and $p = -\frac{d\sigma}{dV}$. giving: $\frac{d}{dV}\left(\frac{d\sigma}{dV}\right) = \frac{B}{V}$. Then, by an integration, one gets:

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

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

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

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

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

Therefore, from Equations (6) and (7), one obtains the expressions for relative dielectric constant $\varepsilon(r_{d(a)}, x)$ and energy band gap $E_{gn(gp)}(r_{d(a)}, x)$, as:

(i)-for $r_{d(a)} \geq r_{do(ao)}$, since $\varepsilon(r_{d(a)}, x) = \frac{\varepsilon_o(x)}{\sqrt{1+\left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3}} \leq \varepsilon_o(x)$, being a **new** **$\varepsilon(r_{d(a)}, x)$-law**,

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

according to the increase in both $E_{gn(gp)}(r_{d(a)}, x)$ and $E_{d(a)}(r_{d(a)}, x)$, with increasing $r_{d(a)}$ and for a given x, and

(ii)-for $r_{d(a)} \leq r_{do(ao)}$, since $\varepsilon(r_{d(a)}, x) = \frac{\varepsilon_o(x)}{\sqrt{1-\left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3}} \geq \varepsilon_o(x)$, with a condition, given by: $\left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 < 1$, being a **new $\varepsilon(r_{d(a)}, x)$-law**,

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

corresponding to the decrease in both $E_{gn(gp)}(r_{d(a)}, x)$ and $E_{d(a)}(r_{d(a)}, x)$, with decreasing $r_{d(a)}$ and for a given x; therefore, the effective Bohr radius $a_{Bn(Bp)}(r_{d(a)}, x)$ is defined by:

$$a_{Bn(Bp)}(r_{d(a)}, x) \equiv \frac{\varepsilon(r_{d(a)}, x) \times \hbar^2}{m_{c(v)}(x) \times q^2} = 0.53 \times 10^{-8}\ \text{cm} \times \frac{\varepsilon(r_{d(a)}, x)}{m_{c(v)}(x)/m_o}. \quad (8c)$$

Furthermore, it is interesting to remark that the critical total donor (acceptor)-density in the metal-insulator transition (**MIT**) at T=0 K, $N_{CDn(NDp)}(r_{d(a)}, x)$, was given by the Mott's criterium, with an empirical parameter, $M_{n(p)}$, as:

$$N_{CDn(CDp)}(r_{d(a)}, x)^{1/3} \times a_{Bn(Bp)}(r_{d(a)}, x) = M_{n(p)},\ M_{n(p)} = 0.25, \quad (9a)$$

depending thus on our **new $\varepsilon(r_{d(a)}, x)$-law.**

This excellent one can be explained from the definition of the reduced effective Wigner-Seitz (**WS**) radius $r_{sn(sp)}$, characteristic of interactions, by:

$$r_{sn(sp)}(N, r_{d(a)}, x) \equiv \left(\frac{3}{4\pi N}\right)^{1/3} \times \frac{1}{a_{Bn(Bp)}(r_{d(a)}, x)} = 1.1723 \times 10^8 \times \left(\frac{1}{N}\right)^{1/3} \times \frac{m_{c(v)}(x)/m_o}{\varepsilon(r_{d(a)}, x)}, \quad (9b)$$

being equal to, in particular, at N=$N_{CDn(CDp)}(r_{d(a)},x)$: $r_{sn(sp)}\left(N_{CDn(CDp)}(r_{d(a)},x), r_{d(a)},x\right)$= **2.4814**, for any $(r_{d(a)},x)$-values. So, from Eq. (9b), one also has:

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

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

Furthermore, by using $\mathbf{M}_{\mathbf{n(p)}} = \mathbf{0.25}$, according to the empirical Heisenberg parameter $\mathcal{H}_{\mathbf{n(p)}} = \mathbf{0.47137}$, as those given in Equations (8, 15) of the Ref.[1], we have also showed that $N_{CDn(CDp)}$ is just the density of electrons (holes) localized in the exponential conduction (valence)-band tail, with a precision of the order of 2.91×10^{-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:

$$E_{gni(gpi)}(r_{d(a)},x,T) \text{ in eV} = E_{gno(gpo)}(r_{d(a)},x) - 10^{-4} \times T^2 \times \left\{\frac{5.405\times x}{T+204\text{ K}} + \frac{3.065\times(1-x)}{T+94\text{ K}}\right\}, \quad (10)$$

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 $m_r(x)/m_o$ is the reduced effective mass $m_r(x)/m_o$, defined by :
$m_r(x) \equiv [m_c(x) \times m_v(x)]/[m_c(x) + m_v(x)]$.

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

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

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

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

where u is the reduced electron density, $u(N, r_{d(a)}, x, T) \equiv \frac{N^*}{N_{c(v)}(T,x)}$,

$F(u) = au^{\frac{2}{3}}\left(1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}}\right)^{-\frac{2}{3}}$, $a = \left[(3\sqrt{\pi}/4) \times u\right]^{2/3}$, $b = \frac{1}{8}\left(\frac{\pi}{a}\right)^2$, $c = \frac{62.3739855}{1920}\left(\frac{\pi}{a}\right)^4$,

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) $\frac{E_{Fn}(u \ll 1)}{k_B T}\left(\frac{-E_{Fp}(u \ll 1)}{k_B T}\right) \ll -1$, 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, $E_{cn(cp)}\left(N, r_{d(a)}, x\right)$, is given as:

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

Then, taking into account various spin-polarized chemical potential-energy contributions such as: exchange energy of an effective electron (hole) gas, majority-carrier correlation energy of an effective electron (hole) gas, minority hole (electron) correlation energy, majority electron (hole)-ionized d(a) interaction screened Coulomb potential energy, and finally minority hole (electron)-ionized d(a) interaction screened Coulomb potential energy, the band gap narrowings are given in the following.

In the n-type HD X(x)- alloy, the BGN is found to be given by:

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

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

$$\Delta E_{gn}(N, r_d, x) = \Delta E_{gno}(N, r_d, x) \times \{2 \times x + 6 \times (1 - x)\}, \quad (14n)$$

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:

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

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

$$\Delta E_{gp}(N, r_a, x) = \Delta E_{gpo}(N, r_a, x) \times \{2 \times x + 6 \times (1 - x)\}, \quad (14p)$$

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]

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

$$\varepsilon_1 \equiv n^2 - \kappa^2 \text{ and } \varepsilon_2 \equiv 2n\kappa, \quad (16)$$

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

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

, for a=1, (18)

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

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

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

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

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

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

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

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

going to a constant as $E \to \infty$, since $n(E \to \infty, r_{d(a)}, x) \to n_\infty(r_{d(a)}, x) = \sqrt{\varepsilon(r_{d(a)}, x)} \times \frac{\omega_T}{\omega_L}$, $\omega_T = 5.1 \times 10^{13}\ s^{-1}$ [5] and $\omega_L = 8.9755 \times 10^{13}\ s^{-1}$.

Here, the other parameters are determined by: $X_i(E_{gn1(gp1)}) = \frac{A_i}{Q_i} \times \left[-\frac{B_i^2}{2} + E_{gn1(gp1)} B_i - E_{gn1(gp1)}^2 + C_i\right]$,

$Y_i(E_{gn1(gp1)}) = \frac{A_i}{Q_i} \times \left[\frac{B_i \times (E_{gn1(gp1)}^2 + C_i)}{2} - 2E_{gn1(gp1)} C_i\right]$, $Q_i = \frac{\sqrt{4C_i - B_i^2}}{2}$, where, for i=(1, 2, 3, and 4), $A_i = 1.154 \times A_{i(FB)} = 4.7314 \times 10^{-4},\ 0.2314, 0.1118$ and 0.0116, $B_i \equiv B_{i(FB)} = 5.871, 6.154, 9.679$ and 13.232, and $C_i \equiv C_{i(FB)} = 8.619, 9.784, 23.803$, and 44.119.

Then, as noted above, if the two optical functions, n and κ, are both known, the other ones defined in Equations (16, 17) can also be determined.

NUMERICAL RESULTS

Now, some numerical results of those optical functions are investigated in the n(p)-type $\mathbf{X(x) \equiv GaTe_{1-x}P_x}$- 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 $R_\infty(r_{d(a)}, x)$ go to their appropriate limiting constants for T=0K, 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 [$\geq E_{CPE}(r_{P(B)}, x)$] 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 $\mathbf{X(x) \equiv GaTe_{1-x}P_x}$- 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 2.91×10^{-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	Te	Sb	Sn
r_d (nm) [4]	↗	0.110	0.132	0.136	0.140
At **x=0**,					
E_{CPE} in meV	↗	1791.7	1796	1796.1	1796.6
n_{MIT}	↘	3.315	3.178	3.174	3.161
$\varepsilon_{1(MIT)}$	↘	10.99	10.10	10.07	9.99
R_{MIT}	↘	0.288	0.272	0.271	0.2697
At **x=0.5**,					
E_{CPE} in meV	↗	1792.1	1796	1796.1	1796.6
n_{MIT}	↘	3.263	3.129	3.125	3.112
$\varepsilon_{1(MIT)}$	↘	10.64	9.79	9.76	9.68
R_{MIT}	↘	0.282	0.266	0.265	0.264
At **x=1**,					
E_{CPE} in meV	↗	1792.7	1796	1796.1	1796.5
n_{MIT}	↘	3.208	3.078	3.074	3.062
$\varepsilon_{1(MIT)}$	↘	10.29	9.47	9.45	9.38
R_{MIT}	↘	0.275	0.2597	0.2592	0.2577
Acceptor		B	Ga	In	Cd
r_a (nm)	↗	0.088	0.126	0.144	0.148
At **x=0**,					
E_{CPE} in meV	↗	1770.5	1796	1803	1807
n_{MIT}	↘	3.917	3.178	3.086	3.045

$\varepsilon_{1(MIT)}$	↘	15.34	10.10	9.522	9.271
R_{MIT}	↘	0.352	0.272	0.261	0.255
At **x=0.5**,					
E_{CPE} in meV	↗	1764.2	1796	1805	1809.4
n_{MIT}	↘	3.853	3.129	3.038	2.997
$\varepsilon_{1(MIT)}$	↘	14.85	9.79	9.23	8.98
R_{MIT}	↘	0.346	0.266	0.255	0.250
At **x=1**,					
E_{CPE} in meV	↗	1756.8	1796	1807	1812.5
n_{MIT}	↘	3.789	3.078	2.988	2.948
$\varepsilon_{1(MIT)}$	↘	14.36	9.47	8.93	8.69
R_{MIT}	↘	0.339	0.260	0.248	0.243

Table 2: Here, as T=0K and N=$N_{CDn(p)}(r_{d(a)}, x)$, and for $E \to \infty$ 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	Te	Sb	Sn
At **x=0**,					
n_{∞}	↘	2.1277	1.9928	1.9886	1.9762
$\varepsilon_{1,\infty}$	↘	4.5269	3.9712	3.9547	3.9053
$\sigma_{O,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	9.7087	9.0933	9.0743	9.0174
$\propto_{\infty}$ in $(10^9 \times cm^{-1})$=		2.1602			
R_{∞}	↘	0.1300	0.1100	0.1094	0.1076
At **x=0.5**,					
n_{∞}	↘	2.0751	1.9436	1.9395	1.9274
$\varepsilon_{1,\infty}$	↘	4.3061	3.7775	3.7618	3.7148

$\sigma_{o,\infty}$ in $\frac{10^5}{\Omega\times cm}$ ↘	9.4689	8.8687	8.8502	8.7947
$\propto_\infty$ in $(10^9 \times cm^{-1})$=	2.1602			
R_∞ ↘	0.1222	0.1027	0.1021	0.1003
At **x=1**,				
n_∞ ↘	2.0212	1.8931	1.8891	1.8773
$\varepsilon_{1,\infty}$ ↘	4.0853	3.5838	3.5689	3.5343
$\sigma_{o,\infty}$ in $\frac{10^5}{\Omega\times cm}$ ↘	9.2229	8.6383	8.6203	8.5663
$\propto_\infty$ in $(10^9 \times cm^{-1})$=	2.1602			
R_∞ ↘	0.1142	0.0953	0.0947	0.0930
Acceptor	B	Ga	In	Cd
At **x=0**,				
n_∞ ↘	2.716	1.993	1.905	1.866
$\varepsilon_{1,\infty}$ ↘	7.374	3.971	3.629	3.483
$\sigma_{o,\infty}$ in $\frac{10^5}{\Omega\times cm}$ ↘	12.39	9.093	8.693	8.517
$\propto_\infty$ in $(10^9 \times cm^{-1})$=	2.160			
R_∞ ↘	0.213	0.110	0.097	0.091
At **x=0.5**,				
n_∞ ↘	2.648	1.943	1.858	1.820
$\varepsilon_{1,\infty}$ ↘	7.014	3.777	3.452	3.314
$\sigma_{o,\infty}$ in $\frac{10^5}{\Omega\times cm}$ ↘	12.08	8.869	8.478	8.306
$\propto_\infty$ in $(10^9 \times cm^{-1})$=	2.160			
R_∞ ↘	0.204	0.103	0.090	0.085
At **x=1**,				
n_∞ ↘	2.580	1.893	1.810	1.773
$\varepsilon_{1,\infty}$ ↘	6.655	3.584	3.275	3.144
$\sigma_{o,\infty}$ in $\frac{10^5}{\Omega\times cm}$ ↘	11.77	8.64	8.26	8.09

$\propto_{\infty}$ in $(10^9 \times cm^{-1})$=2.160				
R_{∞} ↘	0.195	0.095	0.083	0.078

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,				
$\mathbf{E_{CPE} = 1.7917}$	**3.3156**	**0**	**10.993**	**0**
2	3.462	0.187	11.949	1.296
2.5	3.992	0.190	15.898	1.516
3	4.176	1.199	15.999	10.016
3.5	3.640	1.520	10.938	11.062
4	3.771	1.476	12.044	11.134
4.5	4.085	2.387	10.992	19.502
5	2.609	3.441	−5.032	17.955
5.5	1.534	2.487	−3.832	7.632
6	1.616	1.888	−0.952	6.103
…				
$\mathbf{10^{22}}$	**2.1277**	**0**	**4.5269**	**0**
At x=0.5,				
$\mathbf{E_{CPE}}$ **=1.7921**	**3.7632**	**0**	**10.6455**	**0**
2	3.408	0.187	11.583	1.276
2.5	3.938	0.190	15.474	1.494
3	4.123	1.198	15.559	9.881
3.5	3.587	1.519	10.559	10.896
4	3.718	1.475	11.650	10.974
4.5	4.032	2.386	10.567	19.244
5	2.557	3.440	−5.296	17.590

5.5	1.482	2.487	−3.987	7.371
6	1.564	1.887	−1.116	5.904
…				
10^{22}	**2.0751**	**0**	**4.3061**	**0**
At x=1,				
E_{CPE} =1.7927	**3.2084**	**0**	**10.2943**	**0**
2	3.354	0.187	11.213	1.254
2.5	3.883	0.189	15.044	1.471
3	4.068	1.197	15.114	9.741
3.5	3.533	1.518	10.177	10.724
4	3.664	1.475	11.253	10.808
4.5	3.978	2.385	10.137	18.977
5	2.503	3.439	−5.558	17.214
5.5	1.429	2.486	−4.138	7.103
6	1.511	1.887	−1.279	5.701
…				
10^{22}	**2.0212**	**0**	**4.0853**	**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} =1.7705	**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	4.368	1.505	16.814	13.144
4.5	4.685	2.424	16.073	22.717
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**
At x=0.5,				
E_{CPE} =1.7642	**3.8535**	**0**	**14.8494**	**0**
2	4.021	0.195	16.133	1.565
2.5	4.565	0.205	20.799	1.871
3	4.736	1.254	20.853	11.881
3.5	4.171	1.569	14.934	13.086
4	4.303	1.530	16.229	13.022
4.5	4.621	2.435	15.427	22.511
5	3.118	3.500	−2.529	21.823
5.5	2.028	2.524	−2.256	10.241
6	2.115	1.912	0.814	8.089
…				
10^{22}	**2.6485**	**0**	**7.0146**	**0**
At x=1,				
E_{CPE} =1.7568	**3.7893**	**0**	**14.3590**	**0**
2	3.963	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 $\eta_n(\gg 1, \text{degenerate case})$, E_{gn1}, n, κ, ε_1 and ε_2, obtained as functions of N, being represented by the arrows: ↗ and ↘, noting that both η_n and E_{gn1} increase with increasing N.

N (10^{18} cm^{-3})	↗	15	26	60	100
			x=0		
For $\mathbf{r_d} = \mathbf{r_{Te}}$,					
$\eta_n \gg 1$	↗	234	340	599	844
E_{gn1} in eV	↗	1.672	1.711	1.854	2.026
n	↘	3.994	3.956	3.815	3.641
κ	↘	1.730	1.643	1.342	1.022
ε_1	↘	12.958	12.951	12.751	12.210
ε_2	↘	13.820	13.000	10.241	7.445
For $\mathbf{r_d} = \mathbf{r_{Sb}}$,					
$\eta_n \gg 1$	↗	233	340	599	844
E_{gn1} in eV	↗	1.673	1.713	1.857	2.029
n	↘	3.989	3.950	3.808	3.633
κ	↘	1.728	1.640	1.337	1.016
ε_1	↘	12.925	12.918	12.713	12.166
ε_2	↘	13.783	12.954	10.186	7.387
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↗	233	340	599	844
E_{gn1} in eV	↗	1.676	1.717	1.864	2.039

n	↘	3.973	3.933	3.788	3.610
κ	↘	1.720	1.630	1.322	0.999
ε_1	↘	12.826	12.817	12.601	12.036
ε_2	↘	13.671	12.821	10.020	7.216

x=0.5

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

$\eta_n \gg 1$	↗	129	187	328		462
E_{gn1} in eV	↘	1.597	1.579	1.575	↗	1.599
n	↗	4.017	4.034	4.038	↘	4.015
κ	↗	1.906	1.948	1.958	↘	1.901
ε_1	↘	12.508	12.480	12.473	↗	12.510
ε_2	↗	15.311	15.715	15.818	↘	15.264

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

$\eta_n \gg 1$	↗	129	187	328		462
E_{gn1} in eV	↘	1.598	1.580	1.577	↗	1.602
n	↗	4.012	4.029	4.032	↘	4.008
κ	↗	1.903	1.944	1.953	↘	1.894
ε_1	↘	12.476	12.450	12.444	↗	12.482
ε_2	↗	15.273	15.668	15.751	↘	15.182

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

$\eta_n \gg 1$	↗	129	187	328		462
E_{gn1} in eV	↘	1.601	1.584	1.583	↗	1.610
n	↗	3.997	4.013	4.014	↘	3.988
κ	↗	1.896	1.935	1.937	↘	1.873
ε_1	↘	12.383	12.359	12.357	↗	12.396
ε_2	↗	15.161	15.527	15.552	↘	14.940

x=1

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

$\eta_n \gg 1$	↗	93		135		236		331
E_{gn1} in eV	↘	1.678		1.671	↗	1.678		1.704
n	↗	3.889		3.896	↘	3.888		3.863
κ	↗	1.718		1.734	↘	1.716		1.658
ε_1	↘	12.173		12.171	↗	12.173		12.174
ε_2	↗	13.364		13.511	↘	13.346		12.808

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

$\eta_n \gg 1$	↗	93		135		236		331
E_{gn1} in eV	↘	1.678		1.671	↗	1.680		1.707
n	↗	3.884		3.891	↘	3.883		3.857
κ	↗	1.716		1.732	↘	1.713		1.653
ε_1	↘	12.143		12.141	↗	12.143		12.1431
ε_2	↗	13.336		13.477	↘	13.300		12.754

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

$\eta_n \gg 1$	↗	93		135		236		331
E_{gn1} in eV		1.680	↘	1.674	↗	1.684		1.713
n		3.871	↗	3.876	↘	3.866		3.839
κ		1.712	↗	1.725	↘	1.702		1.640
ε_1		12.051	↘	12.050	↗	12.052	↘	12.051
ε_2	↗	13.254		13.377	↘	13.165		12.593
N (10^{18} cm^{-3})	↗	15		26		60		100

Table 4p: In the X(x)-system, at E=3.2 eV and T=20 K, for given r_d and x, and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of $\eta_p(\gg 1, \text{degenerate case})$, E_{gp1}, n, κ, ε_1 and ε_2, obtained as functions of N, being represented by the arrows: ↗ and ↘, noting that both η_p and E_{gp1} increase with increasing N.

$N\ (10^{18}\ cm^{-3})$	↗	15	26	60	100
x=0					
For $\mathbf{r_a} = \mathbf{r_{Ga}}$,					
$\eta_p \gg 1$	↗	199	312	578	826
E_{gp1} in eV	↗	2.001	2.150	2.516	2.871
n	↘	3.666	3.511	3.112	2.723
κ	↘	1.066	0.818	0.346	0.080
ε_1	↘	12.306	11.661	9.566	7.302
ε_2	↘	7.820	5.743	2.155	0.434
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↗	186	302	570	820
E_{gp1} in eV	↗	1.997	2.152	2.528	2.889
n	↘	3.582	3.421	3.012	2.594
κ	↘	1.073	0.814	0.335	0.072
ε_1	↘	11.683	11.042	8.958	6.725
ε_2	↘	7.688	5.573	2.016	0.372
For $\mathbf{r_a} = \mathbf{r_{Cd}}$,					
$\eta_p \gg 1$	↗	178	296	566	816
E_{gp1} in eV	↗	1.993	2.151	2.532	2.896
n	↘	3.548	3.383	2.969	2.547
κ	↘	1.079	0.815	0.331	0.069
ε_1	↘	11.421	10.782	8.703	6.485

ε_2	↘	7.659	5.517	1.965	0.349

x=0.5

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

$\eta_p \gg 1$	↗	93	158	307	445
E_{gp1} in eV	↗	1.888	1.973	2.179	2.376
n	↘	3.732	3.645	3.431	3.219
κ	↘	1.277	1.115	0.772	0.503
ε_1	↘	12.299	12.044	11.175	10.108
ε_2	↘	9.530	8.133	5.301	3.240

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

$\eta_p \gg 1$	↗	80	149	300	439
E_{gp1} in eV	↗	1.882	1.973	2.185	2.386
n	↘	3.652	3.560	3.339	3.122
κ	↘	1.287	1.116	0.763	0.491
ε_1	↘	11.680	11.428	10.565	9.505
ε_2	↘	9.401	7.946	5.096	3.064

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

$\eta_p \gg 1$	↗	72	143	296	435
E_{gp1} in eV	↗	1.878	1.972	2.187	2.390
n	↘	3.619	3.524	3.299	3.080
κ	↘	1.295	1.118	0.760	0.486
ε_1	↘	11.416	11.166	10.305	9.249
ε_2	↘	9.377	7.883	5.015	2.993

x=1

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

$\eta_p \gg 1$	↗	47	99	210	310

E_{gp1} in eV	↗	1.854	1.930	2.099	2.255
n	↘	3.716	3.638	3.464	3.299
κ	↘	1.343	1.195	0.898	0.661
ε_1	↘	12.001	11.811	11.196	10.447
ε_2	↘	9.983	8.696	6.221	4.364

For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↗	28	87	202	303
E_{gp1} in eV	↗	1.838	1.924	2.100	2.259
n	↘	3.648	3.561	3.380	3.211
κ	↘	1.376	1.207	0.897	0.656
ε_1	↘	11.418	11.228	10.622	9.884
ε_2	↘	10.039	8.597	6.063	4.213

For $\mathbf{r_a} = \mathbf{r_{Cd}}$,					
$\eta_p \gg 1$	↗	13	80	197	300
E_{gp1} in eV	↗	1.824	1.919	2.100	2.260
n	↘	3.626	3.530	3.344	3.173
κ	↘	1.404	1.216	0.898	0.654
ε_1	↘	11.174	10.980	10.378	9.643
ε_2	↘	10.184	8.582	6.004	4.152
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 $\mathbf{r_d} = \mathbf{r_{Te}}$,

$\eta_n \gg 1$	↘	844	338	169	56
E_{gn1} in eV	↘	2.026	2.021	2.011	1.956
n	↗	3.641	3.645	3.656	3.712
κ	↗	1.022	1.030	1.048	1.147
ε_1	↗	12.210	12.227	12.267	12.463
ε_2	↗	7.445	7.508	7.665	8.512

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

$\eta_n \gg 1$	↘	844	338	169	56
E_{gn1} in eV	↘	2.029	2.025	2.014	1.960
n	↗	3.633	3.638	3.648	3.704
κ	↗	1.016	1.024	1.042	1.140
ε_1	↗	12.166	12.183	12.224	12.421
ε_2	↗	7.387	7.449	7.606	8.449

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

$\eta_n \gg 1$	↘	844	337	169	56
E_{gn1} in eV	↘	2.039	2.035	2.024	1.970
n	↗	3.610	3.615	3.626	3.682
κ	↗	0.999	1.007	1.025	1.122
ε_1	↗	12.036	12.053	12.095	12.295
ε_2	↗	7.216	7.278	7.432	8.263

x=0.5

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

$\eta_n \gg 1$	↘	462	185	92.4	31
E_{gn1} in eV	↘	1.599	1.594	1.583	1.516
n	↗	4.015	4.019	4.030	4.094
κ	↗	1.901	1.911	1.938	2.103
ε_1	↘	12.510	12.504	12.487	12.338

ε_2	↗	15.264	15.362	15.626	17.216

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

$\eta_n \gg 1$	↘	462	185	92.4	31
E_{gn1} in eV	↘	1.601	1.597	1.586	1.519
n	↗	4.008	4.013	4.024	4.087
κ	↗	1.894	1.904	1.931	2.095
ε_1	↘	12.482	12.476	12.459	12.313
ε_2	↗	15.182	15.280	15.543	17.128

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

$\eta_n \gg 1$	↘	462	185	92.4	31
E_{gn1} in eV	↘	1.610	1.606	1.595	1.527
n	↗	3.988	3.992	4.003	4.067
κ	↗	1.873	1.883	1.911	2.074
ε_1	↘	12.396	12.390	12.375	12.238
ε_2	↗	14.940	15.037	15.297	16.866

x=1

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

$\eta_n \gg 1$	↘	331	133	66	22
E_{gn1} in eV	↘	1.704	1.700	1.688	1.608
n	↗	3.863	3.867	3.879	3.956
κ	↗	1.658	1.667	1.695	1.879
ε_1	↗	12.1739	12.1745	12.1747 ↘	12.1205
ε_2	↗	12.808	12.897	13.155	14.864

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

$\eta_n \gg 1$	↘	331	133	66	22
E_{gn1} in eV	↘	1.707	1.702	1.690	1.610
n	↗	3.857	3.861	3.873	3.950
κ	↗	1.653	1.663	1.691	1.874

ε_1	↗	12.1431	12.1438	12.1442 ↘	12.0919
ε_2	↗	12.754	12.843	13.100	14.804
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↘	331	133	66	22
E_{gn1} in eV	↘	1.713	1.708	1.696	1.616
n	↗	3.839	3.843	3.856	3.932
κ	↗	1.640	1.650	1.677	1.860
ε_1	↗	12.0506	12.0516	12.0528 ↘	12.0061
ε_2	↗	12.593	12.681	12.936	14.627
T in K	↗	20	50	100	300

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

T in K	↗	20	50	100	300
			x=0		
For $\mathbf{r_a} = \mathbf{r_{Ga}}$,					
$\eta_p \gg 1$	↘	826	331	165	55
E_{gp1} in eV	↘	2.871	2.866	2.856	2.801
n	↗	2.703	2.708	2.721	2.785
κ	↗	0.080	0.082	0.088	0.118
ε_1	↗	7.302	7.329	7.396	7.744
ε_2	↗	0.434	0.446	0.477	0.656
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↘	820	328	164	55
E_{gp1} in eV	↘	2.889	2.884	2.874	2.819

n	↗	2.594	2.599	2.612	2.676
κ	↗	0.072	0.074	0.079	0.107
ε_1	↗	6.725	6.751	6.816	7.151
ε_2	↗	0.372	0.383	0.411	0.574

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

$\eta_p \gg 1$	↘	816	327	163	54
E_{gp1} in eV	↘	2.896	2.891	2.881	2.826
n	↗	2.547	2.552	2.565	2.629
κ	↗	0.069	0.070	0.075	0.103
ε_1	↗	6.485	6.510	6.573	6.904
ε_2	↗	0.349	0.360	0.387	0.544

x=0.5

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

$\eta_p \gg 1$	↘	445	178	89	30
E_{gp1} in eV	↘	2.376	2.372	2.360	2.293
n	↗	3.219	3.223	3.236	3.309
κ	↗	0.503	0.509	0.523	0.610
ε_1	↗	10.108	10.133	10.200	10.578
ε_2	↗	3.240	3.279	3.384	4.036

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

$\eta_p \gg 1$	↘	439	175	88	29
E_{gp1} in eV	↘	2.386	2.382	2.370	2.303
n	↗	3.122	3.127	3.139	3.212
κ	↗	0.491	0.496	0.510	0.596
ε_1	↗	9.505	9.530	9.595	9.964
ε_2	↗	3.064	3.101	3.202	3.829

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

$\eta_p \gg 1$	↘	435	174	87	29
E_{gp1} in eV	↘	2.390	2.386	2.374	2.307
n	↗	3.080	3.083	3.097	3.170
κ	↗	0.486	0.491	0.505	0.591
ε_1	↗	9.249	9.273	9.337	9.702
ε_2	↗	2.993	3.030	3.129	3.745

x=1

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

$\eta_p \gg 1$	↘	310	124	62	21
E_{gp1} in eV	↘	2.255	2.251	2.238	2.159
n	↗	3.299	3.304	3.317	3.402
κ	↗	0.661	0.667	0.685	0.803
ε_1	↗	10.447	10.470	10.535	10.928
ε_2	↗	4.364	4.411	4.547	5.467

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

$\eta_p \gg 1$	↘	303	121	61	20
E_{gp1} in eV	↘	2.259	2.255	2.242	2.163
n	↗	3.211	3.216	3.230	3.314
κ	↗	0.656	0.662	0.680	0.797
ε_1	↗	9.884	9.906	9.969	10.350
ε_2	↗	4.213	4.258	4.390	5.287

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

$\eta_p \gg 1$	↘	300	120	60	20
E_{gp1} in eV	↘	2.260	2.256	2.244	2.164
n	↗	3.173	3.178	3.192	3.276
κ	↗	0.654	0.660	0.678	0.796
ε_1	↗	9.643	9.665	9.727	10.102
ε_2	↗	4.152	4.197	4.328	5.214

T in K	↗	20	50	100	300