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OPTICAL COEFFICIENTS IN THE N(P)-TYPE DEGENERATE GaTe(1-x) As(x)-CRYSTALLINE ALLOY, DUE TO THE NEW STATIC DIELECTRIC CONSTANT-LAW AND THE GENERALIZED MOTT CRITERIUM IN THE METAL-INSULATOR TRANSITION. (6)

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ABTRACT

In the n(p)-type $GaTe_{1-x}As_x$- crystalline alloy, with $0 \leq x \leq 1$, basing on our two recent works[1,2], for a given x, and with an increasing $r_{d(a)}$, the optical coefficients have been determined, as functions of the photon energy E, total impurity density N, the donor (acceptor) radius $r_{d(a)}$, concentration x, and temperature T. Those results have been affected by **(i)** the important new $\varepsilon(r_{d(a)}, x)$ -law, developed in Equations (8a, 8b), stating that, for a given x, due to the impurity-size effect, ε decreases (↘) with an increasing (↗) $r_{d(a)}$, and then by **(ii)** the generalized Mott critical d(a)-density defined in the metal-insulator transition (MIT), $N_{CDn(NDp)}(r_{d(a)}, x)$, as observed in Equations (8c, 9a). Furthermore, we also showed that $N_{CDn(NDp)}$ is just the density of carriers localized in exponential band tails, with a precision of the order of 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: $GaTe_{1-x}As_x$- crystalline alloy; impurity-size effect; Mott critical impurity density in the MIT, optical coefficients.

INTRODUCTION

Here, basing on our two recent works[1,2] and also other ones[3-8], all the optical coefficients given in the n(p)-type $X(x) \equiv GaTe_{1-x}As_x$ - crystalline alloy, with $0 \leq x \leq 1$, are investigated, as functions of the photon energy E, total impurity density N, the donor (acceptor) radius $r_{d(a)}$, concentration x, and temperature T.

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

ENERGY BAND STUCTURE PARAMETERS

First of all, in the $n^+(p^+) - p(n)$ X(x)- crystalline alloy at T=0 K, we denote the donor (acceptor) d(a)-radius by $r_{d(a)}$, and also the intrinsic one by: $r_{do(ao)} = r_{Te(Ga)}$=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:

$$m_{c(v)}(x)/m_o = 0.066(0.291) \times x + 0.209\ (0.4) \times (1-x) \qquad (1)$$

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

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

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

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

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

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

and then, the isothermal bulk modulus, by:

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

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:

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

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

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

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

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

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** $\boldsymbol{\varepsilon(r_{d(a)},x)}$**-law**,

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Furthermore, by using $\mathbf{M}_{n(p)} = \mathbf{0.25}$, according to the empirical Heisenberg parameter $\boldsymbol{\mathcal{H}}_{n(p)} = \mathbf{0.47137}$, as those given in Equations (8, 15) of the Ref.[1], we have also showed that $N_{CDn(CDp)}$ is just the density of electrons (holes) localized in the exponential conduction (valence)-band tail, with a precision of the order of $\mathbf{2.91 \times 10^{-7}}$. 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:

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

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:

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

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 $r_{d(a)}$

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

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

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

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

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

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

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

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

the correlation energy of an effective electron gas, $E_{cn(cp)}(N, r_{d(a)}, x)$, is given as:

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

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

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

$$\Delta E_{gn}(N, r_d, x) \simeq a_1 \times \frac{\varepsilon_o(x)}{\varepsilon(r_d, x)} \times N_r^{1/3} + a_2 \times \frac{\varepsilon_o(x)}{\varepsilon(r_d, x)} \times N_r^{\frac{1}{3}} \times (2.503 \times [-E_{cn}(r_{sn}) \times r_{sn}]) + a_3 \times \left[\frac{\varepsilon_o(x)}{\varepsilon(r_d, x)}\right]^{5/4} \times \sqrt{\frac{m_v}{m_r}} \times N_r^{1/4} + a_4 \times \sqrt{\frac{\varepsilon_o(x)}{\varepsilon(r_d, x)}} \times N_r^{1/2} \times 2 + a_5 \times \left[\frac{\varepsilon_o(x)}{\varepsilon(r_d, x)}\right]^{\frac{3}{2}} \times N_r^{\frac{1}{6}}, \quad N_r \equiv \left(\frac{N^*}{N_{CDn}(r_d, x)}\right), \tag{14n}$$

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

$$\Delta E_{gp}(N, r_a, x) \simeq a_1 \times \frac{\varepsilon_o(x)}{\varepsilon(r_a, x)} \times N_r^{1/3} + a_2 \times \frac{\varepsilon_o(x)}{\varepsilon(r_a, x)} \times N_r^{\frac{1}{3}} \times (2.503 \times [-E_{cp}(r_{sp}) \times r_{sp}]) + a_3 \times \left[\frac{\varepsilon_o(x)}{\varepsilon(r_a, x)}\right]^{5/4} \times \sqrt{\frac{m_c}{m_r}} \times N_r^{1/4} + 2a_4 \times \sqrt{\frac{\varepsilon_o(x)}{\varepsilon(r_a, x)}} \times N_r^{1/2} + a_5 \times \left[\frac{\varepsilon_o(x)}{\varepsilon(r_a, x)}\right]^{\frac{3}{2}} \times N_r^{\frac{1}{6}}, \quad N_r \equiv \left(\frac{N^*}{N_{CDp}(r_a, x)}\right), \tag{14p}$$

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

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:

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

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)≡ $\sum_{i=1}^{4}\frac{A_i}{E^2 - B_i E + C_i}$ and F(E)≡ $\sum_{i=1}^{4}\frac{A_i}{E^2\times(1+10^{-4}\times\frac{E}{6}) - B_i E + C_i}$, we propose:

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

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

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 $X(x) \equiv GaTe_{1-x}As_x$- crystalline alloy, as follows.

A. Metal-insulator transition (MIT)-case

As discussed above, the physical conditions used for the MIT are found to be given by: T=0K, $N^* = 0$ or $N = N_{CDn(CDp)}$, giving rise to: $E_{gn1(gp1)}(N^* = 0, r_{d(a)}, x, T = 0) = E_{gn1(gp1)}(r_{d(a)}, x) = E_{gno(gpo)}(r_{d(a)}, x)$.

Then, in this MIT-case, if $E = E_{gn1(gp1)}(r_{d(a)}, x) = E_{gno(gpo)}(r_{d(a)}, x)$, which can be defined as the critical photon energy: $E \equiv E_{CPE}(r_{d(a)}, x)$, one obtains: $\kappa_{MIT}(r_{d(a)}, x) = 0$ from Eq. (20), and from Eq. (16): $\varepsilon_{2(MIT)}(r_{d(a)}, x) = 0$, $\sigma_{O(MIT)}(r_{d(a)}, x) = 0$ and $\alpha_{MIT}(r_{d(a)}, x) = 0$, 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 → ∞

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 $\eta_{n(p)} (\gg 1$, 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 $X(x) \equiv GaTe_{1-x}As_x$- crystalline alloy, by basing on our two recent works[1,2], for a given x, and with an increasing $r_{d(a)}$, the optical coefficients have been determined, as functions of the photon energy E, total impurity density N, the donor (acceptor) radius $r_{d(a)}$, concentration x, and temperature T.

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

Further, we also showed that $N_{CDn(NDp)}$ is just the density of carriers localized in exponential band tails, with a precision of the order of 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	0.271	0.270	0.2697
At **x=0.5**,					
E_{CPE} in meV	↗	1655.3	1658	1658.1	1658.4
n_{MIT}	↘	3.436	3.297	3.293	3.280
$\varepsilon_{1(MIT)}$	↘	11.81	10.87	10.84	10.76
R_{MIT}	↘	0.301	0.286	0.285	0.2838
At **x=1**,					
E_{CPE} in meV	↗	1518.8	1520	1520.04	1520.18
n_{MIT}	↘	3.556	3.416	3.412	3.399
$\varepsilon_{1(MIT)}$	↘	12.65	11.673	11.64	11.55
R_{MIT}	↘	0.315	0.299	0.2988	0.297
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	↗	1637.4	1658	1664	1667
n_{MIT}	↘	4.045	3.297	3.204	3.163
$\varepsilon_{1(MIT)}$	↘	16.36	10.87	10.27	10.01
R_{MIT}	↘	0.364	0.286	0.275	0.270
At **x=1**,					
E_{CPE} in meV	↗	1503.7	1520	1524	1527
n_{MIT}	↘	4.173	3.416	3.323	3.281
$\varepsilon_{1(MIT)}$	↘	17.41	11.67	11.04	10.77
R_{MIT}	↘	0.376	0.299	0.289	0.284

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	3.9052
$\sigma_{O,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	9.7087	9.0933	9.0743	9.0174
α_{∞} in $(10^9 \times cm^{-1})$		2.1602	2.1602	2.1602	2.1602
R_{∞}	↘	0.1230	0.1100	0.1094	0.1076
At **x=0.5**,					
n_{∞}	↘	2.1632	2.0261	2.0219	2.0092
$\varepsilon_{1,\infty}$	↘	4.6797	4.1052	4.0881	4.0370
$\sigma_{O,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	9.8711	9.2454	9.2261	9.1683

$\propto_\infty$ in $(10^9 \times cm^{-1})$	2.1602	2.1602	2.1602	2.1602
R_∞ ↘	0.1352	0.1150	0.1142	0.1125
At **x=1**,				
n_∞ ↘	2.1983	2.0589	2.0546	2.0418
$\varepsilon_{1,\infty}$ ↘	4.8324	4.2392	4.2216	4.1688
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega\times cm}$ ↘	10.0309	9.3951	9.3755	9.3167
$\propto_\infty$ in $(10^9 \times cm^{-1})$	2.1602	2.1602	2.1602	2.1602
R_∞ ↘	0.1404	0.1198	0.1192	0.1173

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
$\sigma_{0,\infty}$ 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	2.160	2.160	2.160
R_∞ ↘	0.213	0.110	0.097	0.091
At **x=0.5**,				
n_∞ ↘	2.761	2.026	1.937	1.898
$\varepsilon_{1,\infty}$ ↘	7.623	4.105	3.752	3.601
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega\times cm}$ ↘	12.60	9.245	8.838	8.659
$\propto_\infty$ in $(10^9 \times cm^{-1})$	2.160	2.160	2.160	2.160
R_∞ ↘	0.219	0.115	0.102	0.096
At **x=1**,				
n_∞ ↘	2.806	2.059	1.968	1.928
$\varepsilon_{1,\infty}$ ↘	7.872	4.239	3.874	3.719
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega\times cm}$ ↘	12.80	9.395	8.981	8.799
$\propto_\infty$ in $(10^9 \times cm^{-1})$	2.160	2.160	2.160	2.160
R_∞ ↘	0.225	0.120	0.106	0.100

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**	**10.9930**	**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,				
$\mathbf{E_{CPE} = 1.6553}$	**3.4361**	**0**	**11.8069**	**0**
2	3.696	0.214	13.612	1.581
2.5	4.296	0.270	18.385	2.321
3	4.407	1.485	17.214	13.090
3.5	3.722	1.772	10.716	13.191
4	3.860	1.664	12.128	12.845
4.5	4.196	2.633	10.672	22.098
5	2.580	3.740	−7.328	19.294
5.5	1.433	2.673	−5.093	7.664
6	1.537	2.012	−1.686	6.186
…				
$\mathbf{10^{22}}$	**2.1632**	**0**	**4.6797**	**0**
At x=1,				

E_{CPE} =1.5188	**3.5562**	**0**	**12.6467**	**0**
2	3.943	0.222	15.501	1.752
2.5	4.618	0.364	21.194	3.366
3	4.640	1.802	18.285	16.725
3.5	3.795	2.044	10.224	15.513
4	3.940	1.863	12.055	14.686
4.5	4.302	2.892	10.140	24.881
5	2.540	4.051	−9.959	20.579
5.5	1.320	2.867	−6.474	7.571
6	1.448	2.141	−2.485	6.201
…				
10^{22}	**2.1983**	**0**	**4.8324**	**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} =1.6374	**4.0450**	**0**	**16.3625**	**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}	**2.7610**	**0**	**7.6231**	**0**
At x=1,				
E_{CPE} =1.5037	**4.1730**	**0**	**17.4142**	**0**
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	15.106	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**
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	↗	2.110	2.270	2.665	3.046
n	↘	3.553	3.383	2.943	2.493
κ	↘	0.881	0.641	0.212	0.018
ε_1	↘	11.848	11.035	8.618	6.215
ε_2	↘	6.258	4.338	1.247	0.088
For $\mathbf{r_d} = \mathbf{r_{Sb}}$,					
$\eta_n \gg 1$	↗	233	340	599	844
E_{gn1} in eV	↗	2.110	2.270	2.666	3.046
n	↘	3.549	3.379	2.938	2.488
κ	↘	0.881	0.641	0.211	0.017
ε_1	↘	11.818	11.005	8.590	6.190
ε_2	↘	6.247	4.329	1.243	0.087
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↗	233	340	599	844
E_{gn1} in eV	↗	2.111	2.271	2.667	3.048
n	↘	3.535	3.365	2.924	2.473
κ	↘	0.879	0.639	0.210	0.017
ε_1	↘	11.726	10.915	8.507	6.116
ε_2	↘	6.215	4.302	1.229	0.084
x=0.5					

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

$\eta_n \gg 1$	↗	130	188	329	463
E_{gn1} in eV	↗	1.725	1.781	1.930	2.083
n	↘	3.976	3.921	3.772	3.615
κ	↘	1.613	1.493	1.195	0.925
ε_1	↘	13.208	13.147	12.797	12.211
ε_2	↘	12.827	11.710	9.014	6.691

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

$\eta_n \gg 1$	↗	130	188	329	463
E_{gn1} in eV	↗	1.725	1.781	1.931	2.084
n	↘	3.971	3.916	3.766	3.609
κ	↘	1.612	1.492	1.193	0.923
ε_1	↘	13.174	13.113	12.762	12.175
ε_2	↘	12.802	11.684	8.987	6.665

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

$\eta_n \gg 1$	↗	130	188	329	463
E_{gn1} in eV	↗	1.727	1.783	1.934	2.088
n	↘	3.957	3.902	3.750	3.593
κ	↘	1.608	1.487	1.187	0.917
ε_1	↘	13.072	13.011	12.657	12.066
ε_2	↘	12.728	11.606	8.907	6.588

x=1

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

$\eta_n \gg 1$	↗	93.6	135	236	332
E_{gn1} in eV	↘	1.234	1.174	1.068	0.998

n	↗	4.466	4.519	4.611	4.671
κ	↗	2.865	3.042	3.368	3.596
ε_1	↘	11.740	11.169	9.915	8.890
ε_2	↗	25.596	27.494	31.063	33.592

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

$\eta_n \gg 1$	↗	93.6	135	236	332
E_{gn1} in eV	↘	1.235	1.176	1.071	1.002
n	↗	4.461	4.513	4.604	4.663
κ	↗	2.861	3.036	3.359	3.582
ε_1	↘	11.715	11.151	9.916	8.912
ε_2	↗	25.523	27.402	30.927	33.416

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

$\eta_n \gg 1$	↗	94	135	236	332
E_{gn1} in eV	↘	1.240	1.182	1.081	1.013
n	↗	4.444	4.495	4.583	4.640
κ	↗	2.847	3.018	3.330	3.544
ε_1	↘	11.640	11.097	9.919	8.973
ε_2	↗	25.307	27.129	30.522	32.894

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 ↗ 2.115 2.303 2.746 3.161

---

n ↘ 3.548 3.348 2.850 2.351

κ ↘ 0.872 0.597 0.153 0.001

ε_1 ↘ 11.825 10.852 8.102 5.528

ε_2 ↘ 6.191 3.997 0.873 0.005

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

$\eta_p \gg 1$ ↗ 186 302 570 820

E_{gp1} in eV ↗ 2.101 2.294 2.742 3.161

---

n ↘ 3.474 3.270 2.766 2.264

κ ↘ 0.894 0.609 0.155 0.001

ε_1 ↘ 11.271 10.320 7.630 5.124

ε_2 ↘ 6.218 3.981 0.860 0.005

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

$\eta_p \gg 1$ ↗ 178 296 566 816

E_{gp1} in eV ↗ 2.093 2.288 2.740 3.160

---

n ↘ 3.444 3.237 2.731 2.226

κ ↘ 0.908 0.616 0.157 0.001

ε_1 ↘ 11.039 10.099 7.432 4.956

ε_2 ↘ 6.259 3.989 0.857 0.005

---

x=0.5

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

$\eta_p \gg 1$ ↗ 118 178 322 457

E_{gp1} in eV $\nearrow$ 1.830 1.924 2.152 2.369

---

n $\searrow$ 3.872 3.778 3.542 3.309

κ $\searrow$ 1.391 1.206 0.814 0.512

ε_1 $\searrow$ 13.060 12.816 11.883 10.686

ε_2 $\searrow$ 10.776 9.116 5.764 3.386

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

$\eta_p \gg 1$ $\nearrow$ 114 175 319 455

E_{gp1} in eV $\nearrow$ 1.831 1.927 2.157 2.376

---

n $\searrow$ 3.782 3.686 3.447 3.212

κ $\searrow$ 1.389 1.201 0.805 0.503

ε_1 $\searrow$ 12.375 12.142 11.234 10.064

ε_2 $\searrow$ 10.510 8.856 5.554 3.232

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

$\eta_p \gg 1$ $\nearrow$ 112 173 318 454

E_{gp1} in eV $\nearrow$ 1.831 1.928 2.160 2.379

---

n $\searrow$ 3.743 3.645 3.405 3.169

κ $\searrow$ 1.389 1.199 0.802 0.499

ε_1 $\searrow$ 12.080 11.851 10.954 9.796

ε_2 $\searrow$ 10.400 8.746 5.463 3.166

---

x=1

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

$\eta_p \gg 1$ $\nearrow$ 89 131 233 329

E_{gp1} in eV $\nearrow$ 1.630 1.691 1.842 1.987

---

n $\searrow$ 4.100 4.042 3.893 3.747

κ $\searrow$ 1.826 1.687 1.367 1.091

ε_1 13.478 $\nearrow$ 13.488 $\searrow$ 13.289 12.847

ε_2 $\searrow$ 14.974 13.638 10.648 8.173

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

$\eta_p \gg 1$	↗	87	130	232	329
E_{gp1} in eV	↗	1.635	1.697	1.850	1.996
n	↘	4.005	3.945	3.795	3.646
κ	↘	1.815	1.674	1.352	1.074
ε_1		12.746 ↗	12.762 ↘	12.575	12.142
ε_2	↘	14.543	13.213	10.259	7.830

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

$\eta_p \gg 1$	↗	86	129	232	328
E_{gp1} in eV	↗	1.637	1.700	1.853	2.001
n	↘	3.963	3.903	3.751	3.602
κ	↘	1.811	1.669	1.345	1.066
ε_1		12.430 ↗	12.449 ↘	12.266	11.837
ε_2	↘	14.353	13.026	10.089	7.680

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	↘	3.046	3.041	3.031	2.976

n	↗	2.493	2.498	2.511	2.577
κ	↗	0.018	0.019	0.021	0.037
ε_1	↗	6.215	6.241	6.305	6.640
ε_2	↗	0.088	0.093	0.106	0.191

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

$\eta_n \gg 1$	↘	844	338	169	56
E_{gn1} in eV	↘	3.046	3.042	3.032	2.977
n	↗	2.488	2.493	2.506	2.572
κ	↗	0.017	0.018	0.021	0.037
ε_1	↗	6.190	6.216	6.280	6.614
ε_2	↗	0.087	0.092	0.105	0.189

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

$\eta_n \gg 1$	↘	844	337	169	56
E_{gn1} in eV	↘	3.048	3.044	3.034	2.979
n	↗	2.473	2.478	2.491	2.577
κ	↗	0.017	0.018	0.020	0.036
ε_1	↗	6.116	6.142	6.205	6.538
ε_2	↗	0.084	0.089	0.102	0.185

---

x=0.5

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

$\eta_n \gg 1$	↘	463	185	92	31
E_{gn1} in eV	↘	2.083	2.078	2.067	2.000
n	↗	3.615	3.619	3.631	3.701
κ	↗	0.925	0.933	0.952	1.068
ε_1	↗	12.211	12.231	12.281	12.555
ε_2	↗	6.691	6.751	6.913	7.904

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

$\eta_n \gg 1$	↘	463	185	92	31
E_{gn1} in eV	↘	2.084	2.080	2.068	2.001
n	↗	3.609	3.614	3.626	3.695
κ	↗	0.923	0.930	0.950	1.066
ε_1	↗	12.175	12.194	12.245	12.519
ε_2	↗	6.665	6.725	6.887	7.875

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

$\eta_n \gg 1$	↘	463	185	92	31
E_{gn1} in eV	↘	2.088	2.083	2.072	2.005
n	↗	3.593	3.597	3.609	3.678
κ	↗	0.917	0.924	0.943	1.059
ε_1	↗	12.066	12.086	12.136	12.411
ε_2	↗	6.588	6.648	6.808	7.789

x=1

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

$\eta_n \gg 1$	↘	331.9	132.8	66	22
E_{gn1} in eV	↘	0.998	0.993	0.981	0.901
n	↗	4.671	4.675	4.685	4.752
κ	↗	3.596	3.610	3.651	3.918
ε_1	↘	8.890	8.822	8.622	7.230
ε_2	↗	33.592	33.753	34.214	37.233

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

$\eta_n \gg 1$	↘	331.9	132.8	66	22
E_{gn1} in eV	↘	1.002	0.997	0.985	0.905
n	↗	4.663	4.667	4.678	4.744
κ	↗	3.583	3.597	3.638	3.904
ε_1	↘	8.912	8.844	8.645	7.264
ε_2	↗	33.416	33.576	34.036	37.045

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

$\eta_n \gg 1$	↘	331.9	132.7	66	22
E_{gn1} in eV	↘	1.013	1.009	0.996	0.917
n	↗	4.640	4.644	4.655	4.721
κ	↗	3.544	3.558	3.599	3.864
ε_1	↘	8.973	8.907	8.713	7.362
ε_2	↗	32.894	33.053	33.508	36.487
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	↘	3.161	3.157	3.147	3.092
n	↗	2.351	2.356	2.369	2.436
κ	↗	0.001	0.00136	0.00211	0.008632
ε_1	↗	5.528	5.552	5.614	5.937
ε_2	↗	0.005	0.00641	0.00999	0.042
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↘	820	328	164	54.6
E_{gp1} in eV	↘	3.161	3.157	3.146	3.0918
n	↗	2.264	2.269	2.282	2.349
κ	↗	0.00112	0.00138	0.00213	0.008681
ε_1	↗	5.124	5.148	5.207	5.518

ε_2	↗	0.00507	0.00626	0.00974	0.0408
For $\mathbf{r_a} = \mathbf{r_{Cd}}$,					
$\eta_p \gg 1$	↘	816	327	163	54.4
E_{gp1} in eV	↘	3.160	3.156	3.145	3.091
n	↗	2.226	2.231	2.244	2.312
κ	↗	0.00117	0.00144	0.00220	0.00882
ε_1	↗	4.956	4.979	5.037	5.343
ε_2	↗	0.00522	0.00641	0.00989	0.04079

x=0.5

For $\mathbf{r_a} = \mathbf{r_{Ga}}$,					
$\eta_p \gg 1$	↘	457	183	91	30
E_{gp1} in eV	↘	2.369	2.365	2.353	2.286
n	↗	3.309	3.313	3.326	3.399
κ	↗	0.512	0.517	0.531	0.619
ε_1	↗	10.686	10.712	10.781	11.170
ε_2	↗	3.386	3.426	3.535	4.207
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↘	455	182	91	30
E_{gp1} in eV	↘	2.376	2.372	2.360	2.293
n	↗	3.212	3.217	3.229	3.302
κ	↗	0.503	0.508	0.523	0.609
ε_1	↗	10.064	10.089	10.155	10.533
ε_2	↗	3.232	3.271	3.376	4.026
For $\mathbf{r_a} = \mathbf{r_{Cd}}$,					
$\eta_p \gg 1$	↘	454	181	90.7	30
E_{gp1} in eV	↘	2.379	2.375	2.363	2.296
n	↗	3.169	3.174	3.187	3.260

κ	↗	0.499	0.505	0.520	0.605
ε_1	↗	9.796	9.820	9.886	10.259
ε_2	↗	3.166	3.204	3.307	3.948

x=1

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

$\eta_p \gg 1$	↘	329	132	66	22
E_{gp1} in eV	↘	1.987	1.983	1.970	1.890
n	↗	3.747	3.751	3.764	3.845
κ	↗	1.091	1.099	1.121	1.271
ε_1	↗	12.847	12.864	12.910	13.166
ε_2	↗	8.173	8.242	8.442	9.775

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

$\eta_p \gg 1$	↘	328.6	131	65.7	21.8
E_{gp1} in eV	↘	1.996	1.992	1.979	1.900
n	↗	3.646	3.651	3.663	3.744
κ	↗	1.074	1.081	1.104	1.253
ε_1	↗	12.142	12.158	12.203	12.451
ε_2	↗	7.830	7.897	8.090	9.383

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

$\eta_p \gg 1$	↘	328.2	131	65.6	21.8
E_{gp1} in eV	↘	2.001	1.996	1.984	1.904
n	↗	3.602	3.606	3.619	3.700
κ	↗	1.066	1.074	1.096	1.245
ε_1	↗	11.837	11.853	11.897	12.143
ε_2	↗	7.680	7.746	7.937	9.211
T in K	↗	20	50	100	300