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OPTICAL COEFFICIENTS IN THE N(P)-TYPE DEGENERATE GaTe(1-x) Sb(x)-CRYSTALLINE ALLOY, DUE TO THE NEW STATIC DIELECTRIC CONSTANT-LAW AND THE GENERALIZED MOTT CRITERIUM IN THE METAL-INSULATOR TRANSITION. (7)

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ABTRACT

In the n(p)-type $GaTe_{1-x}Sb_x$- 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 2.87×10^{-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: $GaTe_{1-x}Sb_x$- 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 $\mathbf{X(x) \equiv GaTe_{1-x}Sb_x}$ - 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:

$$m_{c(v)}(x)/m_o = 0.047(0.3) \times x + 0.209\ (0.4) \times (1-x) \quad (1)$$

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

$$\varepsilon_o(x) = 15.69 \times x + 12.3 \times (1-x). \quad (2)$$

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

$$E_{go}(x) = 0.81 \times x + 1.796 \times (1-x). \quad (3)$$

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

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

and then, the isothermal bulk modulus, by:

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

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

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

At $r_{d(a)} = r_{do(ao)}$, the needed boundary conditions are found to be, for the impurity-atom volume $V = (4\pi/3)\times\left(r_{d(a)}\right)^3$, $V_{do(ao)} = (4\pi/3)\times\left(r_{do(ao)}\right)^3$, 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:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

being equal to, in particular, at $N{=}N_{CDn(CDp)}(r_{d(a)}, x)$: $r_{sn(sp)}(N_{CDn(CDp)}(r_{d(a)}, x), r_{d(a)}, x)$= **2.4814**, 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 $\boldsymbol{\mathcal{H}}_{\mathbf{n(p)}} = \mathbf{0.47137}$, 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 $\mathbf{2.87} \times \mathbf{10^{-7}}$. 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:

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

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, $u(N, r_{d(a)}, x, T) \equiv \frac{N^*}{N_{c(v)}(T, x)}$, $F(u) = au^{\frac{2}{3}}\left(1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}}\right)^{-\frac{2}{3}}$, $a = [(3\sqrt{\pi}/4) \times u]^{2/3}$, $b = \frac{1}{8}\left(\frac{\pi}{a}\right)^2$, $c = \frac{62.3739855}{1920}\left(\frac{\pi}{a}\right)^4$, 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:

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

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

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

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

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

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

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

$$\Delta E_{gn}(N, r_d, x) = \Delta E_{gno}(N, r_d, x) \times \{0.2 \times x + 6 \times (1 - x)\}, \quad (14n)$$

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:

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

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

$$\Delta E_{gp}(N, r_a, x) = \Delta E_{gpo}(N, r_a, x) \times \{0.2 \times x + 6 \times (1 - x)\}, \quad (14p)$$

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]

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

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

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

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

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

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

Then, one has:

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

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

, for a=1, (18)

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

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

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

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

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

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

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

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

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

Here, the other parameters are determined by:

$X_i\left(E_{gn1(gp1)}\right) = \frac{A_i}{Q_i} \times \left[-\frac{B_i^2}{2} + E_{gn1(gp1)} B_i - E_{gn1(gp1)}^2 + C_i\right]$,

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

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

NUMERICAL RESULTS

Now, some numerical results of those optical functions are investigated in the n(p)-type $\mathbf{X(x) \equiv GaTe_{1-x}Sb_x}$- 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:

$E_{gn1(gp1)}\left(N^* = 0, r_{d(a)}, x, T = 0\right) = E_{gn1(gp1)}\left(r_{d(a)}, x\right) = E_{gno(gpo)}\left(r_{d(a)}, x\right)$.

Then, in this MIT-case, if $E = E_{gn1(gp1)}\left(r_{d(a)}, x\right) = E_{gno(gpo)}\left(r_{d(a)}, x\right)$, which can be defined as the critical photon energy: $E \equiv E_{CPE}\left(r_{d(a)}, x\right)$, one obtains: $\kappa_{MIT}\left(r_{d(a)}, x\right) = 0$ from Eq. (20), and from Eq. (16): $\varepsilon_{2(MIT)}\left(r_{d(a)}, x\right) = 0$, $\sigma_{O(MIT)}\left(r_{d(a)}, x\right) = 0$ and $\propto_{MIT}\left(r_{d(a)}, x\right) = 0$, and the other functions such as : $n_{MIT}\left(r_{d(a)}, x\right)$ from Eq. (21), and $\varepsilon_{1(MIT)}\left(r_{d(a)}, x\right)$ and $R_{MIT}\left(r_{d(a)}, x\right)$ 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: $n\left(E \to \infty, r_{d(a)}, x, T\right) = n_{\infty}\left(r_{d(a)}, x\right) = \sqrt{\varepsilon\left(r_{d(a)}, x\right)} \times \frac{\omega_T}{\omega_L}$, $\omega_T = 5.1 \times 10^{13}\ s^{-1}$ [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: $\kappa_{\infty}\left(r_{d(a)}, x\right) \to 0$ and $\varepsilon_{2,\infty}\left(r_{d(a)}, x\right) \to 0$, as E^{-1}, so that $\varepsilon_{1,\infty}\left(r_{d(a)}, x\right)$, $\sigma_{O,\infty}\left(r_{d(a)}, x\right)$, $\alpha_{\infty}\left(r_{d(a)}, x\right)$ and $R_{\infty}\left(r_{d(a)}, x\right)$ 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 $N = N_{CDn(CDp)}\left(r_{P(B)}, x\right)$, 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 [$\geq E_{CPE}\left(r_{P(B)}, x\right)$] 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 $\mathbf{X(x) \equiv GaTe_{1-x}Sb_x}$ - 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 2.87×10^{-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	↗	1300.9	1303	1303.07	1303.3
n_{MIT}	↘	3.763	3.618	3.614	3.600
$\varepsilon_{1(MIT)}$	↘	14.16	13.09	13.06	12.96
R_{MIT}	↘	0.336	0.321	0.3209	0.3195
At **x=1**,					
E_{CPE} in meV	↗	809.4	810	810.02	810.09
n_{MIT}	↘	4.203	4.050	4.046	4.031
$\varepsilon_{1(MIT)}$	↘	17.66	16.40	16.37	16.25
R_{MIT}	↘	0.379	0.365	0.364	0.363
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	↗	1285.7	1303	1307.8	1310.3
n_{MIT}	↘	4.400	3.618	3.521	3.479
$\varepsilon_{1(MIT)}$	↘	19.36	13.09	12.40	12.10
R_{MIT}	↘	0.396	0.321	0.311	0.306
At **x=1**,					
E_{CPE} in meV	↗	798.2	810	813.3	815
n_{MIT}	↘	4.874	4.050	3.949	3.904
$\varepsilon_{1(MIT)}$	↘	23.75	16.40	15.60	15.24
R_{MIT}	↘	0.435	0.365	0.355	0.351

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_∞	↘	2.2695	2.1257	2.1212	2.1079
$\varepsilon_{1,\infty}$	↘	5.1508	4.5185	4.4997	4.4434
$\sigma_{O,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	10.3560	9.6996	9.6794	9.6187

$\propto_{\infty}$ in $(10^9 \times cm^{-1})$	2.1602	2.1602	2.1602	2.1602
R_{∞} ↘	0.1508	0.1297	0.1290	0.1271
x=1,				
n_{∞} ↘	2.4030	2.2507	2.2460	2.2319
$\varepsilon_{1,\infty}$ ↘	5.7746	5.0658	5.0446	4.9816
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$ ↘	10.9652	10.2702	10.2488	10.1845
$\propto_{\infty}$ in $(10^9 \times cm^{-1})$	2.1602	2.1602	2.1602	2.1602
R_{∞} ↘	0.1700	0.1480	0.1473	0.1453

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
x=0.5,				
n_{∞} ↘	2.897	2.126	2.032	1.991
$\varepsilon_{1,\infty}$ ↘	8.390	4.518	4.129	3.963
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$ ↘	13.22	9.700	9.272	9.084
$\propto_{\infty}$ in $(10^9 \times cm^{-1})$	2.160	2.160	2.160	2.160
R_{∞} ↘	0.237	0.130	0.116	0.110
At **x=1**,				
n_{∞} ↘	3.067	2.251	2.152	2.108
$\varepsilon_{1,\infty}$ ↘	9.407	5.066	4.629	4.444
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$ ↘	13.99	10.27	9.818	9.619
$\propto_{\infty}$ in $(10^9 \times cm^{-1})$	2.160	2.160	2.160	2.160
R_{∞} ↘	0.258	0.148	0.133	0.127

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,		
$E_{CPE} = 1.7917$	**2.1277**	**0**	**4.5269**	**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
…				
10^{22}	**2.1277**	**0**	**4.5269**	**0**
At x=0.5,				
E_{CPE} =1.3009	**3.7632**	**0**	**14.1618**	**0**
2	4.383	0.212	19.166	1.860
2.5	5.183	0.544	26.568	5.642
3	5.034	2.371	19.719	23.874
3.5	3.907	2.518	8.921	19.674
4	4.070	2.205	11.705	17.950
4.5	4.476	3.330	8.943	29.811
5	2.471	4.574	−14.812	22.609
5.5	1.133	3.189	−8.886	7.227
6	1.303	2.354	−3.843	6.134
…				
10^{22}	**2.2695**	**0**	**5.1508**	**0**

=1,

E_{CPE} =0.8094	**4.2030**	**0**	**17.6654**	**0**
2	5.479	0.136	30.005	1.489
2.5	6.594	1.082	42.308	14.270
3	5.921	3.942	19.516	46.676
3.5	4.043	3.769	2.136	30.481
4	4.270	3.081	8.738	26.315
4.5	4.798	4.432	3.378	42.533
5	2.198	5.870	−29.627	25.809
5.5	0.579	3.979	−15.501	4.607
6	0.863	2.872	−7.504	4.957
…				
10^{22}	**2.4030**	**0**	**5.7746**	**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 $\kappa \rightarrow 0$ and $\varepsilon_2 \rightarrow 0$ as $E \rightarrow \infty$.

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} =1.2857	**4.3998**	**0**	**19.3582**	**0**
2	5.037	0.211	25.329	2.123
2.5	5.846	0.558	33.868	6.527
3	5.684	2.414	26.480	27.441
3.5	4.536	2.553	14.055	23.159
4	4.701	2.230	17.124	20.965
4.5	5.110	3.362	14.807	34.357
5	3.088	4.611	−11.731	28.481
5.5	1.741	3.212	−7.287	11.185
6	1.914	2.369	−1.949	9.070
…				
10^{22}	**2.8966**	**0**	**8.3905**	**0**
At x=1,				
E_{CPE} =0.7982	**4.8740**	**0**	**23.7557**	**0**
2	6.167	0.134	38.019	1.650
2.5	7.289	1.096	51.934	15.984
3	6.602	3.982	27.731	52.581
3.5	4.706	3.801	7.696	35.772
4	4.934	3.103	14.720	30.623
4.5	5.466	4.459	9.991	48.745
5	2.851	5.901	−26.697	33.657
5.5	1.225	3.998	−14.485	9.800
6	1.512	2.884	−6.032	8.725
…				
10^{22}	**3.0670**	**0**	**9.4067**	**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	↗	1.674	1.713	1.857	2.029
n	↘	3.988	3.950	3.808	3.632
κ	↘	1.727	1.639	1.337	1.016
ε_1	↘	12.925	12.918	12.713	12.165
ε_2	↘	13.776	12.948	10.180	7.382
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↗	233	340	599	844
E_{gn1} in eV	↗	1.678	1.719	1.866	2.040
n	↘	3.972	3.932	3.787	3.609
κ	↘	1.717	1.627	1.320	0.997
ε_1	↘	12.826	12.817	12.598	12.031
ε_2	↘	13.644	12.794	9.997	7.197

x=0.5

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

$\eta_n \gg 1$	↗	130	188	329	463
E_{gn1} in eV	↘	0.918	0.845	0.720	0.642
n	↗	4.804	4.864	4.965	5.026
κ	↗	3.858	4.111	4.558	4.849
ε_1	↘	8.192	6.761	3.871	1.748
ε_2	↗	37.071	39.999	45.266	48.746

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

$\eta_n \gg 1$	↗	130	188	329	463
E_{gn1} in eV	↘	0.920	0.847	0.724	0.647
n	↗	4.798	4.858	4.957	5.018
κ	↗	3.852	4.102	4.544	4.830
ε_1	↘	8.183	6.770	3.925	1.846
ε_2	↗	36.963	39.861	45.059	48.478

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

$\eta_n \gg 1$	↗	130	188	329	463
E_{gn1} in eV	↘	0.926	0.855	0.735	0.662
n	↗	4.780	4.839	4.935	4.993
κ	↗	3.832	4.076	4.503	4.775
ε_1	↘	8.158	6.795	4.081	2.132
ε_2	↗	36.641	39.450	44.445	47.683

x=1

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

$\eta_n \gg 1$	↗	93.7	135	236	332
E_{gn1} in eV	↗	0.785	0.801	0.856	0.920
n	↘	5.038	5.026	4.981	4.928
κ	↘	4.324	4.267	4.074	3.853

ε_1	↗	6.686	7.045	8.210	9.437
ε_2	↘	43.576	42.894	40.588	37.974

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

$\eta_n \gg 1$	↗	93.7	135	236	332
E_{gn1} in eV	↗	0.785	0.802	0.857	0.922
n	↘	5.033	5.020	4.975	4.922
κ	↘	4.322	4.264	4.070	3.847
ε_1	↗	6.655	7.018	8.190	9.422
ε_2	↘	43.506	42.815	40.494	37.868

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

$\eta_n \gg 1$	↗	93.7	135	236	332
E_{gn1} in eV	↗	0.787	0.804	0.861	0.927
n	↘	5.017	5.004	4.958	4.903
κ	↘	4.314	4.255	4.056	3.829
ε_1	↗	6.559	6.936	8.131	9.376
ε_2	↘	43.297	42.582	40.213	37.554

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

$\eta_p \gg 1$	↗	121	181	323	458
E_{gp1} in eV	↗	1.403	1.473	1.653	1.831
n	↘	4.381	4.316	4.145	3.971
κ	↘	2.394	2.210	1.774	1.389
ε_1		13.459 ↗	13.740	14.037 ↘	13.839
ε_2	↘	20.978	19.077	14.702	11.035

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

$\eta_p \gg 1$	↗	118		178	322		457
E_{gp1} in eV	↗	1.409		1.483	1.668		1.849
n	↘	4.281		4.213	4.038		3.859
κ	↘	2.376		2.186	1.740		1.352
ε_1		12.680	↗	12.972	13.273	↘	13.064
ε_2	↘	20.349		18.425	14.056		10.436

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

$\eta_p \gg 1$	↗	116		177	321		451
E_{gp1} in eV	↗	1.412		1.486	1.674		1.857
n	↘	4.237		4.169	3.990		3.810
κ	↘	2.369		2.176	1.727		1.336
ε_1		12.342	↗	12.640	12.943	↘	12.729
ε_2	↘	20.080		18.147	13.780		10.182

---

x=1

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

$\eta_p \gg 1$	↗	91	133	234	330
E_{gp1} in eV	↗	0.955	1.024	1.193	1.354
n	↘	4.899	4.840	4.694	4.551
κ	↘	3.736	3.508	2.985	2.526
ε_1	↗	10.037	11.117	13.125	14.325
ε_2	↘	36.607	33.964	28.024	22.994

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

$\eta_p \gg 1$	↗	90	132	234	330
E_{gp1} in eV	↗	0.957	1.027	1.197	1.358
n	↘	4.798	4.739	4.592	4.448
κ	↘	3.729	3.500	2.974	2.515

ε_1	↗	9.114	10.207	12.238	13.455
ε_2	↘	33.781	33.170	27.320	22.378

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

$\eta_p \gg 1$	↗	89	131	233	329
E_{gp1} in eV	↗	0.958	1.028	1.198	1.360
n	↘	4.753	4.694	4.547	4.402
κ	↘	3.725	3.496	2.970	2.510
ε_1	↗	8.715	9.814	11.855	13.080
ε_2	↘	35.416	32.818	27.008	22.104

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	1.023	1.042	1.140
ε_1	↗	12.165	12.182	12.223	12.420
ε_2	↗	7.382	7.445	7.601	8.444

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

$\eta_n \gg 1$	↘	844	337	169	56
E_{gn1} in eV	↘	2.040	2.036	2.025	1.971
n	↗	3.609	3.613	3.624	3.680
κ	↗	0.997	1.004	1.023	1.120
ε_1	↗	12.031	12.048	12.090	12.291
ε_2	↗	7.197	7.259	7.413	8.243

x=0.5

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

$\eta_n \gg 1$	↘	463	185	92.6	31
E_{gn1} in eV	↘	0.642	0.638	0.626	0.559
n	↗	5.026	5.029	5.038	5.090
κ	↗	4.849	4.865	4.909	5.169
ε_1	↘	1.748	1.623	1.284	-0.806
ε_2	↗	48.746	48.943	49.472	52.620

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

$\eta_n \gg 1$	↘	463	185	92.6	31
E_{gn1} in eV	↘	0.647	0.643	0.631	0.564
n	↗	5.018	5.021	5.030	5.082
κ	↗	4.830	4.847	4.891	5.149
ε_1	↘	1.846	1.722	1.385	-0.690
ε_2	↗	48.478	48.674	49.202	52.339

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

$\eta_n \gg 1$	↘	463	185	92.6	31

E_{gn1} in eV	↘	0.662	0.658	0.646	0.579
n	↗	4.993	4.996	5.005	5.057
κ	↗	4.775	4.791	4.835	5.092
ε_1	↘	2.132	2.010	1.681	−0.351
ε_2	↗	47.683	47.877	48.400	51.505

x=1

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

$\eta_n \gg 1$	↘	332	133	66	22
E_{gn1} in eV	↘	0.920	0.916	0.903	0.824
n	↗	4.928	4.931	4.942	5.007
κ	↗	3.853	3.868	3.910	4.186
ε_1	↘	9.437	9.358	9.129	7.546
ε_2	↗	37.974	38.148	38.649	41.920

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

$\eta_n \gg 1$	↘	332	133	66	22
E_{gn1} in eV	↘	0.922	0.917	0.905	0.825
n	↗	4.922	4.925	4.936	5.001
κ	↗	3.847	3.862	3.904	4.180
ε_1	↘	9.422	9.343	9.115	7.536
ε_2	↗	37.868	38.042	38.542	41.808

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

$\eta_n \gg 1$	↘	332	133	66	22
E_{gn1} in eV	↘	0.927	0.923	0.910	0.831
n	↗	4.903	4.907	4.917	4.982
κ	↗	3.829	3.844	3.887	4.162
ε_1	↘	9.376	9.298	9.072	7.506
ε_2	↗	37.554	37.727	38.224	41.472
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 $\mathbf{r_a} = \mathbf{r_{Ga}}$,

$\eta_p \gg 1$	↘	458	183	92	30
E_{gp1} in eV	↘	1.831	1.827	1.815	1.748
n	↗	3.971	3.975	3.987	4.053
κ	↗	1.389	1.398	1.422	1.563
ε_1	↗	13.839	13.848	13.873	13.985
ε_2	↗	11.035	11.117	11.339	12.669

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

$\eta_p \gg 1$	↘	457	183	91	30
E_{gp1} in eV	↘	1.849	1.845	1.834	1.766
n	↗	3.859	3.863	3.875	3.941
κ	↗	1.352	1.361	1.384	1.523
ε_1	↗	13.064	13.073	13.099	13.213
ε_2	↗	10.436	10.515	10.726	12.008

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

$\eta_p \gg 1$	↘	456	182	91	30
E_{gp1} in eV	↘	1.857	1.853	1.841	1.774
n	↗	3.810	3.814	3.826	3.892
κ	↗	1.336	1.345	1.368	1.506
ε_1	↗	12.729	12.739	12.764	12.880
ε_2	↗	10.182	10.259	10.467	11.727

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x=1

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

$\eta_p \gg 1$	↘	330	132	66	22
E_{gp1} in eV	↘	1.354	1.349	1.337	1.257
n	↗	4.551	4.554	4.566	4.637

κ	↗	2.526	2.538	2.573	2.797
ε_1	↘	14.325	14.300	14.228	13.680
ε_2	↗	22.994	23.123	23.496	25.947
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↘	330	132	66	22
E_{gp1} in eV	↘	1.358	1.353	1.341	1.261
n	↗	4.448	4.452	4.463	4.535
κ	↗	2.515	2.527	2.562	2.786
ε_1	↘	13.455	13.430	13.357	12.802
ε_2	↗	22.378	22.504	22.869	25.269
For $\mathbf{r_a} = \mathbf{r_{C□}}$,					
$\eta_p \gg 1$	↘	329	132	66	22
E_{gp1} in eV	↘	1.360	1.355	1.343	1.263
n	↗	4.402	4.406	4.418	4.489
κ	↗	2.510	2.522	2.557	2.781
ε_1	↘	13.080	13.055	12.981	12.424
ε_2	↗	22.104	22.230	22.591	24.968
T in K	↗	20	50	100	300