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OPTICAL COEFFICIENTS IN THE N(P)-TYPE DEGENERATE GaP(1-x) Te(x)-CRYSTALLINE ALLOY, DUE TO THE NEW STATIC DIELECTRIC CONSTANT-LAW AND THE GENERALIZED MOTT CRITERIUM IN THE METAL-INSULATOR TRANSITION (17)

Huynh Van Cong*, Jöelle Sulian and Michel Cayrol

Université de Perpignan Via Domitia, Laboratoire de Mathématiques et Physique (LAMPS), EA 4217, Département de Physique, 52, Avenue Paul Alduy, F-66 860 Perpignan, France.

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***Corresponding Author**
Huynh Van Cong
Université de Perpignan Via Domitia, Laboratoire de Mathématiques et Physique (LAMPS), EA 4217, Département de Physique, 52, Avenue Paul Alduy, F-66 860 Perpignan, France.

ABTRACT

In the n(p)-type $\mathbf{GaP_{1-x}Te_x}$- crystalline alloy, with $0 \leq x \leq 1$, basing on our two recent works[1,2], for a given x, and with an increasing $r_{d(a)}$, the optical coefficients have been determined, as functions of the photon energy E, total impurity density N, the donor (acceptor) radius $r_{d(a)}$, concentration x, and temperature T.

Those results have been affected by **(i)** the important new $\varepsilon(r_{d(a)}, x)$-law, developed in Equations (8a, 8b), stating that, for a given x, due to the impurity-size effect, ε decreases (↘) with an increasing (↗) $r_{d(a)}$, and then by **(ii)** the generalized Mott critical d(a)-density defined in the metal-insulator transition (MIT), $N_{CDn(NDp)}(r_{d(a)}, x)$, as observed in Equations (8c, 9a). Furthermore, we also showed that $N_{CDn(NDp)}$ is just the density of carriers localized in exponential band tails, with a precision of the order of $\mathbf{2.92 \times 10^{-7}}$, 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: $GaP_{1-x}Te_x$- crystalline alloy; impurity-size effect; Mott critical impurity density in the MIT, optical coefficients.

INTRODUCTION

Here, basing on our two recent works[1,2] and also other ones[3-8], all the optical coefficients given in the n(p)-type $\mathbf{X(x) \equiv GaP_{1-x}Te_x}$ - 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: $r_{do(ao)}$=$r_{P(Ga)}$=0.110 nm (0.126 nm).

A. Effect of x- concentration

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

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

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

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

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

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

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

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

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

and then, the isothermal bulk modulus, by:

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

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

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

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

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

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

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

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

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

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:

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

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:

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

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:

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

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:

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

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 $\mathbf{2.92 \times 10^{-7}}$. Therefore, the density of electrons (holes) given in parabolic conduction (valence) bands can be defined, as that given in compensated materials, by:

$$N^{*}(N,r_{d(a)},x) \equiv N - N_{CDn(NDp)}(r_{d(a)},x). \qquad (9d)$$

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:

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

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:

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

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:

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

where u is the reduced electron density, $u(N, r_{d(a)}, x, T) \equiv \frac{N^*}{N_{c(v)}(T,x)}$, $F(u) = au^{\frac{2}{3}}\left(1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}}\right)^{-\frac{2}{3}}$, $a = [(3\sqrt{\pi}/4) \times u]^{2/3}$, $b = \frac{1}{8}\left(\frac{\pi}{a}\right)^2$, $c = \frac{62.3739855}{1920}\left(\frac{\pi}{a}\right)^4$, and $G(u) \simeq Ln(u) + 2^{-\frac{3}{2}} \times u \times e^{-du}$; $d = 2^{3/2}\left[\frac{1}{\sqrt{27}} - \frac{3}{16}\right] > 0$. Therefore, from Eq. (12), the Fermi energies are expressed as functions of variables : $N, r_{d(a)}, x$, and T.

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

Now, in Eq. (9b), in which one replaces $m_{c(v)}(x)$ by $m_r(x)$, the effective Wigner-Seitz radius becomes as:

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

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

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

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

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

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

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

$$\Delta E_{gn}(N, r_d, x) = \Delta E_{gno}(N, r_d, x) \times \{2.1 \times x + 2.2 \times (1 - x)\}, \quad (14n)$$

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:

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

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

$$\Delta E_{gp}(N, r_a, x) = \Delta E_{gpo}(N, r_a, x) \times \{8 \times x + 18 \times (1 - x)\}, \quad (14p)$$

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:

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

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]

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

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

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:

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

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

Then, one has:

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

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

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

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

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

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

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

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

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:

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

$Y_i(E_{gn1(gp1)}) = \frac{A_i}{Q_i} \times \left[\frac{B_i \times (E^2_{gn1(gp1)} + C_i)}{2} - 2E_{gn1(gp1)} C_i\right]$, $Q_i = \frac{\sqrt{4C_i - B_i^2}}{2}$, where, for i=(1, 2, 3, and 4), $A_i = 1.154 \times A_{i(FB)} = 4.7314 \times 10^{-4}, 0.2314, 0.1118 \text{ and } 0.0116$, $B_i \equiv B_{i(FB)} = 5.871, 6.154, 9.679$ 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 $\mathbf{X(x) \equiv GaP_{1-x}Te_x}$- 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 $\propto_{MIT}(r_{d(a)}, x) = 0$, and the other functions such as : $n_{MIT}(r_{d(a)}, x)$ from Eq. (21), and $\varepsilon_{1(MIT)}(r_{d(a)}, x)$ and $R_{MIT}(r_{d(a)}, x)$ from Eq. (16) decrease with increasing $r_{d(a)}$ and E_{CPE}, as those investigated in Table 1 in Appendix 1.

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

In Eq. (21), at any T, the choice of the real refraction index: $n(E \to \infty, r_{d(a)}, x, T) = n_\infty(r_{d(a)}, x) = \sqrt{\varepsilon(r_{d(a)}, x)} \times \frac{\omega_T}{\omega_L}$, $\omega_T = 5.1 \times 10^{13}\ s^{-1}$ [5] and $\omega_L = 8.9755 \times 10^{13}\ s^{-1}$, was obtained from the Lyddane-Sachs-Teller relation[5], from which T(L) represent the transverse (longitudinal) optical phonon modes. Then, from Equations (16, 17, 20), from such the asymptotic behavior ($E \to \infty$), we obtain: $\kappa_\infty(r_{d(a)}, x) \to 0$ and $\varepsilon_{2,\infty}(r_{d(a)}, x) \to 0$, as E^{-1}, so that $\varepsilon_{1,\infty}(r_{d(a)}, x)$, $\sigma_{O,\infty}(r_{d(a)}, x)$,

$\alpha_\infty(r_{d(a)},x)$ and $R_\infty(r_{d(a)},x)$ go to their appropriate limiting constants, as those investigated in Table 2 in Appendix 1, in which T=0K and $N = N_{CDn(CDp)}$.

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

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

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

In the X(x)-system, at E=3.2 eV and T=20 K, for given $r_{d(a)}$ and x, and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of $\eta_{n(p)}(\gg 1, \text{degenerate case})$, $E_{gn1(gp1)}$, n, κ, ε_1 and ε_2, obtained as functions of N, being represented by the arrows: ↗ and ↘, as those tabulated in Tables 4n and 4p in Appendix 1.

E. Variations of various optical coefficients as functions of T

In the X(x)-system, at E=3.2 eV and $N = 10^{20} cm^{-3}$, for given $r_{d(a)}$ and x, and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of $\eta_{n(p)}(\gg 1, \text{degenerate case})$, $E_{gn1(gp1)}$, n, κ, ε_1 and ε_2, obtained as functions of T, being represented by the arrows: ↗ and ↘, as those tabulated in Tables 5n and 5p in Appendix 1.

CONCLUDING REMARKS

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

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

Further, we also showed that $N_{CDn(NDp)}$ is just the density of carriers localized in exponential band tails, with a precision of the order of $\mathbf{2.92 \times 10^{-7}}$, as that given in Table 4 of Ref.[1], according to a definition of the effective density of electrons (holes) given in parabolic conduction (valence) bands by: $N^*(N, r_{d(a)}, x) \equiv N - N_{CDn(NDp)}(r_{d(a)}, x)$, as defined in Eq. (9d).

In summary, due to the new $\varepsilon(r_{d(a)}, x)$-law and to the effective density of electrons (holes) given in parabolic conduction (valence) bands $N^*(N, r_{d(a)}, x)$, for a given x, and with an increasing $r_{d(a)}$, the numerical results of all the optical coefficients, obtained in appropriated physical conditions (E, N, T), and calculated by using Equations (15, 16, 20, 21), are reported in Tables 1, 2, 3n, 3p, 4n, 4p, 5n, and 5p in Appendix 1.

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APPENDIX 1

Table 1. In the MIT-case, T=0K, N=$N_{CDn(p)}(r_{d(a)},x)$, and the critical photon energy $E_{CPE} = E = E_{gno(gpo)}(r_{d(a)},x)$, if $E = E_{gn1(gp1)}(r_{d(a)},x) = E_{CPE}(r_{d(a)},x)$, the numerical results of optical functions such as : $n_{MIT}(r_{d(a)},x)$, obtained from Eq. (21), and those of other ones: $\varepsilon_{1(MIT)}(r_{d(a)},x)$ and $R_{MIT}(r_{d(a)},x)$, from Eq. (16), decrease (↘) with increasing (↗) $r_{d(a)}$ and E_{CPE}.

Donor		P	As	Sb	Sn
r_d (nm) [4]	↗	0.110	0.118	0.136	0.140
At **x=0**,					
E_{CPE} in meV	↗	1796	1796.7	1804	1807
n_{MIT}	↘	3.078	3.055	2.872	2.820
$\varepsilon_{1(MIT)}$	↘	9.47	9.33	8.25	7.95
R_{MIT}	↘	0.260	0.257	0.234	0.227
At **x=0.5**,					
E_{CPE} in meV	↗	1796	1796.8	1805	1809
n_{MIT}	↘	3.129	3.105	2.916	2.863
$\varepsilon_{1(MIT)}$	↘	9.79	9.64	8.51	8.19
R_{MIT}	↘	0.266	0.263	0.239	0.232
At **x=1**,					
E_{CPE} in meV	↗	1796	1796.9	1806.6	1810
n_{MIT}	↘	3.178	3.153	2.960	2.904
$\varepsilon_{1(MIT)}$	↘	10.10	9.94	8.76	8.43
R_{MIT}	↘	0.272	0.269	0.245	0.238

Acceptor		B	Ga	In	Cd
r_a (nm)	↗	0.088	0.126	0.144	0.148
At **x=0**,					
E_{CPE} in meV	↗	1756.8	1796	1807	1812
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
At **x=0.5**,					
E_{CPE} in meV	↗	1764.2	1796	1805	1809
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	↗	1770.5	1796	1803	1807
n_{MIT}	↘	3.917	3.178	3.086	3.045
$\varepsilon_{1(MIT)}$	↘	15.34	10.10	9.52	9.27
R_{MIT}	↘	0.352	0.272	0.261	0.255

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

Donor		P	As	Sb	Sn
At **x=0**,					
n_{∞}	↘	1.893	1.870	1.692	1.642
$\varepsilon_{1,\infty}$	↘	3.584	3.498	2.863	2.695
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	8.638	8.535	7.721	7.491
α_{∞} in $(10^9 \times cm^{-1}) = 2.1602$					
R_{∞}	↘	0.095	0.092	0.066	0.059
At **x=0.5**,					
n_{∞}	↘	1.943	1.920	1.737	1.685
$\varepsilon_{1,\infty}$	↘	3.778	3.687	3.018	2.841
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	8.869	8.762	7.927	7.691
α_{∞} in $(10^9 \times cm^{-1}) = 2.1602$					
R_{∞}	↘	0.103	0.099	0.072	0.065
At **x=1**,					
n_{∞}	↘	1.993	1.969	1.782	1.728
$\varepsilon_{1,\infty}$	↘	3.971	3.877	3.173	2.987
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	9.093	8.984	8.128	7.886
α_{∞} in $(10^9 \times cm^{-1}) = 2.1602$					
R_{∞}	↘	0.110	0.106	0.080	0.071

Acceptor		B	Ga	In	Cd
At **x=0**,					
n_{∞}	↘	2.580	1.893	1.810	1.773
$\varepsilon_{1,\infty}$	↘	6.655	3.584	3.275	3.144
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	11.77	8.64	8.26	8.09
α_{∞} in $(10^9 \times cm^{-1}) = 2.1602$					
R_{∞}	↘	0.195	0.095	0.083	0.078
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 $(10^9 \times cm^{-1}) = 2.1602$					
R_{∞}	↘	0.204	0.103	0.090	0.085
At **x=1**,					
n_{∞}	↘	2.715	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	9.09	8.693	8.517
$\propto_{\infty}$ in $(10^9 \times cm^{-1}) = 2.1602$					
R_{∞}	↘	0.213	0.110	0.097	0.091

Table 3n. In the P-X(x)-system, and at T=0K and $N = N_{CDn}(r_p, x)$, according to the MIT, our numerical results of n, κ, ε_1 and ε_2 are obtained from Equations (21, 20, 16), respectively, and expressed as functions of E $[\geq E_{CPE}(r_p, x)]$ and x, noting that (i) $\kappa = 0$ 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,				
$\mathbf{E_{CPE} = 1.796}$	**3.0783**	**0**	**9.4760**	**0**
2	3.221	0.186	10.341	1.198
2.5	3.749	0.188	14.019	1.407
3	3.935	1.191	14.067	9.371
3.5	3.403	1.512	9.298	10.292
4	3.535	1.470	10.334	10.395
4.5	3.848	2.379	9.148	18.312
5	2.376	3.431	−6.128	16.310
5.5	1.304	2.481	−4.458	6.471
6	1.385	1.884	−1.631	5.219
…				
$\mathbf{10^{22}}$	**1.8931**	**0**	**3.5838**	**0**
At x=0.5,				
$\mathbf{E_{CPE}}$ **=1.796**	**3.1288**	**0**	**9.7894**	**0**
2	3.272	0.186	10.669	1.217
2.5	3.799	0.188	14.400	1.426
3	3.985	1.191	14.467	9.492
3.5	3.454	1.512	9.644	10.444
4	3.585	1.470	10.693	10.544
4.5	3.899	2.379	9.539	18.552
5	2.427	3.431	−5.885	16.656
5.5	1.354	2.481	−4.323	6.721

6	1.436	1.884	-1.488	5.410
…				
10^{22}	**1.9436**	**0**	**3.7775**	**0**
At x=1,				
E_{CPE} =1.796	**3.1780**	**0**	**10.100**	**0**
2	3.321	0.186	10.993	1.235
2.5	3.848	0.188	14.776	1.444
3	4.035	1.191	14.861	9.609
3.5	3.503	1.512	9.986	10.593
4	3.635	1.470	11.049	10.688
4.5	3.948	2.379	9.925	18.786
5	2.476	3.431	-5.644	16.994
5.5	1.403	2.481	-4.188	6.966
6	1.485	1.884	-1.345	5.595
…				
10^{22}	**1.9928**	**0**	**3.9712**	**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} =1.7568	**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	20.267	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	14.969	22.317
5	3.045	3.516	-3.087	21.416
5.5	1.952	2.535	-2.610	9.895
6	2.040	1.919	0.477	7.830
…				
10^{22}	**2.5797**	**0**	**6.6548**	**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	1.513	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} =1.7705	**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**
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 $\mathbf{r_d = r_P}$,					
$\eta_n \gg 1$	↗	123.7	179	313	441
E_{gn1} in eV	↗	1.692	1.700	1.746	1.811
n	↘	3.875	3.868	3.822	3.758
κ	↘	1.685	1.669	1.567	1.430
ε_1	↘	12.1749	12.1746	12.155	12.079
ε_2	↘	13.0618	12.9087	11.982	10.751

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

$\eta_n \gg 1$	↗	122.8	178.4	313	440.7
E_{gn1} in eV	↗	1.740	1.762	1.839	1.930
n	↘	3.627	3.606	3.530	3.438
κ	↘	1.579	1.533	1.374	1.196
ε_1	↘	10.661	10.652	10.573	10.391
ε_2	↘	11.456	11.059	9.700	8.225

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

$\eta_n \gg 1$	↗	122.5	178.1	312.8	440.5
E_{gn1} in eV	↗	1.752	1.777	1.861	1.958
n	↘	3.565	3.541	3.457	3.359
κ	↘	1.554	1.501	1.330	1.144
ε_1	↘	10.295	10.283	10.185	9.976
ε_2	↘	11.080	10.634	9.196	7.685

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x=0.5

For $\mathbf{r_d} = \mathbf{r_P}$,

$\eta_n \gg 1$	↗	103	149	262	369
E_{gn1} in eV	↗	1.745	1.762	1.823	1.896
n	↘	3.874	3.857	3.797	3.724
κ	↘	1.569	1.534	1.406	1.261
ε_1	↘	12.544	12.529	12.441	12.278
ε_2	↘	12.159	11.832	10.679	9.389

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

$\eta_n \gg 1$	↗	101	148	261	368
E_{gn1} in eV	↗	1.782	1.809	1.891	1.983
n	↘	3.631	3.605	3.522	3.429
κ	↘	1.490	1.435	1.269	1.098
ε_1	↘	10.964	10.935	10.794	10.553
ε_2	↘	10.823	10.346	8.942	7.527

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

$\eta_n \gg 1$	↗	101	147.8	261	368
E_{gn1} in eV	↗	1.791	1.820	1.908	2.004
n	↘	3.570	3.541	3.453	3.356
κ	↘	1.471	1.411	1.237	1.060

ε_1	↘	10.582	10.551	10.396	10.136
ε_2	↘	10.502	9.995	8.546	7.115
			x=1		
For $\mathbf{r_d = r_P}$,					
$\eta_n \gg 1$	↗	91	133	235	331
E_{gn1} in eV	↗	1.777	1.799	1.870	1.950
n	↘	3.892	3.869	3.799	3.718
κ	↘	1.501	1.454	1.310	1.159
ε_1	↘	12.892	12.858	12.713	12.485
ε_2	↘	11.685	11.251	9.954	8.617
For $\mathbf{r_d = r_{Sb}}$,					
$\eta_n \gg 1$	↗	89	132	233	330
E_{gn1} in eV	↗	1.808	1.838	1.926	2.019
n	↘	3.650	3.620	3.531	3.436
κ	↘	1.437	1.375	1.204	1.033
ε_1	↘	11.256	11.211	11.022	10.736
ε_2	↘	10.490	9.956	8.501	7.100
For $\mathbf{r_d = r_{Sn}}$,					
$\eta_n \gg 1$	↗	88	131	233	329
E_{gn1} in eV	↗	1.815	1.848	1.939	2.036
n	↘	3.589	3.557	3.464	3.365
κ	↘	1.421	1.356	1.178	1.004
ε_1	↘	10.861	10.813	10.615	10.316
ε_2	↘	10.199	9.644	8.163	6.756
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 $\mathbf{r_a = r_{Ga}}$,					

$\eta_p \gg 1$	↗	63	132	280	413
E_{gp1} in eV	↗	1.700	1.702	1.761	1.843
n	↘	3.867	3.865	3.807	3.726
κ	↘	1.668	1.663	1.534	1.365
ε_1	↘	12.1745	12.1743	12.142	12.023
ε_2	↘	12.899	12.855	11.680	10.173
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↗	37	116	269	404
E_{gp1} in eV	↗	1.726	1.723	1.791	1.882
n	↗	3.759	3.762	↘ 3.694	3.604
κ	↗	1.610	1.618	↘ 1.471	1.287
ε_1	↗	11.5335	11.5344	↘11.485	11.330
ε_2	↗	12.107	12.172	↘10.869	9.278
For $\mathbf{r_a} = \mathbf{r_{Cd}}$,					
$\eta_p \gg 1$	↗	17	106	262	399
E_{gp1} in eV	↗	1.748	1.731	1.803	1.898
n	↗	3.700	3.717	↘ 3.646	3.551
κ	↗	1.562	1.599	↘ 1.446	1.256
ε_1	↗	11.2503	11.2576	↘11.201	11.031
ε_2	↗	11.558	11.890	↘10.542	8.918
x=0.5					
For $\mathbf{r_a} = \mathbf{r_{Ga}}$,					
$\eta_p \gg 1$	↗	74	127	245	355
E_{gp1} in eV	↗	1.701	1.704	1.744	1.804
n	↘	3.916	3.914	3.874	3.816
κ	↘	1.664	1.659	1.570	1.444
ε_1	↘	12.5673	12.5668	12.545	12.473
ε_2	↘	13.038	12.991	12.168	11.024
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↗	64	119	240	350
E_{gp1} in eV	↗	1.720	1.725	1.775	1.843
n	↘	3.812	3.808	3.759	3.692
κ	↘	1.623	1.613	1.505	1.365
ε_1	↘	11.901	11.899	11.863	11.763

ε_2	↘	12.375	12.282	11.318	10.082
For $\mathbf{r_a = r_{Cd}}$,					
$\eta_p \gg 1$	↗	58	114	237	348
E_{gp1} in eV	↗	1.729	1.734	1.788	1.859
n	↘	3.766	3.761	3.708	3.637
κ	↘	1.604	1.593	1.478	1.332
ε_1	↘	11.612	11.610	11.567	11.455
ε_2	↘	12.084	11.983	10.965	9.694
			x=1		
For $\mathbf{r_a = r_{Ga}}$,					
$\eta_p \gg 1$	↗	78	122	226	324
E_{gp1} in eV	↗	1.742	1.757	1.814	1.882
n	↘	3.925	3.911	3.855	3.787
κ	↘	1.575	1.544	1.425	1.287
ε_1	↘	12.9303	12.916	12.834	12.683
ε_2	↘	12.362	12.078	10.986	9.749
For $\mathbf{r_a = r_{In}}$,					
$\eta_p \gg 1$	↗	73	118	223	322
E_{gp1} in eV	↗	1.757	1.774	1.839	1.914
n	↘	3.824	3.807	3.743	3.667
κ	↘	1.544	1.507	1.374	1.226
ε_1	↘	12.237	12.220	12.121	11.944
ε_2	↘	11.810	11.473	10.283	8.991
For $\mathbf{r_a = r_{Cd}}$,					
$\eta_p \gg 1$	↗	70	116	222	320
E_{gp1} in eV	↗	1.763	1.782	1.849	1.928
n	↘	3.779	3.761	3.693	3.614
κ	↘	1.531	1.491	1.352	1.200
ε_1	↘	11.939	11.919	11.812	11.625
ε_2	↘	11.572	11.215	9.986	8.675
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 $\mathbf{r_d = r_P}$,					
$\eta_n \gg 1$	↘	441	176	88	29
E_{gn1} in eV	↘	1.811	1.801	1.776	1.648
n	↗	3.758	3.768	3.793	3.917
κ	↗	1.430	1.451	1.502	1.785
ε_1	↗	12.079	12.094	12.126	12.160
ε_2	↗	10.751	10.935	11.398	13.986
For $\mathbf{r_d = r_{Sb}}$,					
$\eta_n \gg 1$	↘	440.7	176.3	88.1	29.3
E_{gn1} in eV	↘	1.930	1.920	1.895	1.767
n	↗	3.438	3.448	3.473	3.601
κ	↗	1.196	1.215	1.262	1.522
ε_1	↗	10.391	10.415	10.470	10.649
ε_2	↗	8.225	8.380	8.769	10.964
For $\mathbf{r_d = r_{Sn}}$,					
$\eta_n \gg 1$	↘	440.5	176.2	88.09	29.34
E_{gn1} in eV	↘	1.958	1.948	1.923	1.795
n	↗	3.359	3.369	3.394	3.523
κ	↗	1.144	1.162	1.209	1.463
ε_1	↗	9.976	10.002	10.062	10.269
ε_2	↗	7.685	7.833	8.206	10.310
x=0.5					
For $\mathbf{r_d = r_P}$,					
$\eta_n \gg 1$	↘	369	148	74	24.6
E_{gn1} in eV	↘	1.896	1.889	1.870	1.766
n	↗	3.724	3.731	3.750	3.853
κ	↗	1.261	1.275	1.311	1.524
ε_1	↗	12.278	12.296	12.342	12.524

ε_2	↗	9.389	9.512	9.833	11.743

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

$\eta_n \gg 1$	↘	368	147	74	24.5
E_{gn1} in eV	↘	1.983	1.976	1.957	1.853
n	↗	3.429	3.436	3.455	3.560
κ	↗	1.098	1.111	1.145	1.344
ε_1	↗	10.553	10.574	10.629	10.868
ε_2	↗	7.527	7.633	7.910	9.570

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

$\eta_n \gg 1$	↘	368	147	73.6	24.5
E_{gn1} in eV	↘	2.004	1.997	1.978	1.874
n	↗	3.356	3.363	3.382	3.487
κ	↗	1.060	1.073	1.106	1.302
ε_1	↗	10.136	10.158	10.214	10.465
ε_2	↗	7.115	7.216	7.484	9.084

x=1

For $\mathbf{r_d} = \mathbf{r_P}$,

$\eta_n \gg 1$	↘	331	132	66	22
E_{gn1} in eV	↘	1.950	1.945	1.933	1.853
n	↗	3.718	3.723	3.736	3.816
κ	↗	1.159	1.167	1.190	1.344
ε_1	↗	12.485	12.499	12.539	12.753
ε_2	↗	8.617	8.688	8.893	10.261

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

$\eta_n \gg 1$	↘	329.7	131.9	65.9	21.9
E_{gn1} in eV	↘	2.019	2.015	2.002	1.923
n	↗	3.436	3.440	3.453	3.534
κ	↗	1.033	1.041	1.063	1.209
ε_1	↗	10.736	10.751	10.794	11.029
ε_2	↗	7.100	7.162	7.342	8.547

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

$\eta_n \gg 1$	↘	329.3	131.7	65.8	21.9
E_{gn1} in eV	↘	2.036	2.032	2.019	1.940
n	↗	3.365	3.370	3.382	3.464

κ	↗	1.004	1.011	1.033	1.177
ε_1	↗	10.316	10.331	10.374	10.614
ε_2	↗	6.756	6.816	6.990	8.156
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 $\mathbf{r_a = r_{Ga}}$,					
$\eta_p \gg 1$	↘	413	165	82	27
E_{gp1} in eV	↘	1.843	1.833	1.808	1.680
n	↗	3.726	3.736	3.761	3.886
κ	↗	1.365	1.382	1.436	1.712
ε_1	↗	12.023	12.042	12.083	12.174
ε_2	↗	10.173	10.351	10.799	13.310
For $\mathbf{r_a = r_{In}}$,					
$\eta_p \gg 1$	↘	404	161	81	27
E_{gp1} in eV	↘	1.882	1.872	1.847	1.719
n	↗	3.604	3.614	3.638	3.765
κ	↗	1.287	1.307	1.356	1.625
ε_1	↗	11.330	11.352	11.400	11.535
ε_2	↗	9.278	9.446	9.867	12.237
For $\mathbf{r_a = r_{Cd}}$,					
$\eta_p \gg 1$	↘	399	159	80	26
E_{gp1} in eV	↘	1.898	1.888	1.864	1.736
n	↗	3.551	3.561	3.586	3.712
κ	↗	1.256	1.275	1.323	1.590
ε_1	↗	11.031	11.053	11.105	11.256
ε_2	↗	8.918	9.081	9.492	11.803
			x=0.5		

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

$\eta_p \gg 1$	↘	355	142	71	24
E_{gp1} in eV	↘	1.804	1.797	1.778	1.674
n	↗	3.816	3.823	3.841	3.943
κ	↗	1.444	1.459	1.498	1.725
ε_1	↗	12.473	12.484	12.509	12.568
ε_2	↗	11.024	11.158	11.512	13.606

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

$\eta_p \gg 1$	↘	350.5	140	70	23
E_{gp1} in eV	↘	1.843	1.835	1.817	1.713
n	↗	3.692	3.699	3.717	3.819
κ	↗	1.365	1.380	1.418	1.639
ε_1	↗	11.763	11.776	11.808	11.903
ε_2	↗	10.082	10.209	10.542	12.521

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

$\eta_p \gg 1$	↘	348	139	69.5	23
E_{gp1} in eV	↘	1.859	1.852	1.833	1.729
n	↗	3.637	3.645	3.663	3.766
κ	↗	1.332	1.347	1.384	1.603
ε_1	↗	11.455	11.469	11.503	11.612
ε_2	↗	9.694	9.818	10.142	12.072

x=1

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

$\eta_p \gg 1$	↘	324	129	65	21
E_{gp1} in eV	↘	1.882	1.878	1.865	1.786
n	↗	3.787	3.791	3.804	3.883
κ	↗	1.287	1.296	1.320	1.483
ε_1	↗	12.683	12.694	12.725	12.879
ε_2	↗	9.749	9.825	10.046	11.515

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

$\eta_p \gg 1$	↘	321	128	64.3	21
E_{gp1} in eV	↘	1.914	1.910	1.897	1.817
n	↗	3.667	3.671	3.684	3.764

κ	↗	1.226	1.234	1.258	1.417
ε_1	↗	11.944	11.956	11.989	12.159
ε_2	↗	8.991	9.064	9.273	10.666

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

$\eta_p \gg 1$	↘	320	128	64	21
E_{gp1} in eV	↘	1.928	1.923	1.911	1.831
n	↗	3.614	3.619	3.632	3.712
κ	↗	1.200	1.208	1.232	1.389
ε_1	↗	11.625	11.637	11.671	11.847
ε_2	↗	8.675	8.746	8.950	10.311
T in K	↗	20	50	100	300