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OPTICAL COEFFICIENTS IN THE N(P)-TYPE DEGENERATE GaP(1-x) Sb(x)-CRYSTALLINE ALLOY, DUE TO THE NEW STATIC DIELECTRIC CONSTANT-LAW AND THE GENERALIZED MOTT CRITERIUM IN THE METAL-INSULATOR TRANSITION (18)

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ABTRACT

In the n(p)-type $\mathbf{GaP_{1-x}Sb_x}$- 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 $\mathbf{2.92 \times 10^{-7}}$, 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: $GaP_{1-x}Sb_x$- 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 $\mathbf{X(x) \equiv GaP_{1-x}Sb_x}$ - 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:

$$m_{c(v)}(x)/m_o = 0.047\ (0.3) \times x + 0.13(0.5) \times (1-x) \qquad (1)$$

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

$$\varepsilon_o(x) = 15.69 \times x + 11.1 \times (1-x). \qquad (2)$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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 $\mathcal{H}_{\mathbf{n(p)}} = \mathbf{0.47137}$, 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 $\mathbf{2.92 \times 10^{-7}}$. Therefore, the density of electrons (holes) given in parabolic conduction (valence) bands can be defined, as that given in compensated materials, by:

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

C. Effect of temperature T, with given x and $\mathbf{r_{d(a)}}$

Here, the intrinsic band gap $E_{gni(gpi)}(r_{d(a)}, x, T)$ at any T is given by:

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

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

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

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

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

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

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

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

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

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

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

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:

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

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

$$\Delta E_{gn}(N, r_d, x) = \Delta E_{gno}(N, r_d, x) \times \{0.75 \times x + 2.2 \times (1 - x)\}, \quad (14n)$$

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

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

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

$$\Delta E_{gp}(N, r_a, x) = \Delta E_{gpo}(N, r_a, x) \times \{15 \times x + 18 \times (1 - x)\}, \quad (14p)$$

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

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

OPTICAL BAND GAP

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

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

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: $E_{gn1(gp1)}\left(r_{d(a)}, x\right) = E_{gno(gpo)}\left(r_{d(a)}, x\right)$, 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 $E > E_{gn1(gp1)}$,

$$J_{n(p)}(E,N,r_{d(a)},x,T)=\frac{1}{2\pi^2}\times\left(\frac{2m_r}{\hbar^2}\right)^{3/2}\times\frac{(E-E_{gn1(gp1)})^{a-(1/2)}}{E_{gni(gpi)}^{a-1}}=\frac{1}{2\pi^2}\times\left(\frac{2m_r}{\hbar^2}\right)^{3/2}\times\frac{(E-E_{gn1(gp1)})^{2}}{E_{gni(gpi)}^{3/2}}$$, 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)$\equiv\sum_{i=1}^{4}\frac{A_i}{E^2-B_iE+C_i}$ and F(E)$\equiv\sum_{i=1}^{4}\frac{A_i}{E^2\times(1+10^{-4}\times\frac{E}{6})-B_iE+C_i}$, we propose:

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

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

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

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

going to a constant as $E\to\infty$, since $n(E\to\infty,r_{d(a)},x)\to n_\infty(r_{d(a)},x)=\sqrt{\varepsilon(r_{d(a)},x)}\times\frac{\omega_T}{\omega_L}$, $\omega_T=5.1\times10^{13}\ s^{-1}$ [5] and $\omega_L=8.9755\times10^{13}\ s^{-1}$.

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), $A_i=1.154\times A_{i(FB)}=4.7314\times10^{-4}, 0.2314, 0.1118$ 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 $\mathbf{X(x) \equiv GaP_{1-x}Sb_x}$- 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: $E_{gn1(gp1)}(N^* = 0, r_{d(a)}, x, T = 0) = E_{gn1(gp1)}(r_{d(a)}, x) = E_{gno(gpo)}(r_{d(a)}, x)$.

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 $\mathbf{X(x) \equiv GaP_{1-x}Sb_x}$- 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 $\mathbf{2.92 \times 10^{-7}}$, 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	↗	1303	1303.3	1306.8	1308
n_{MIT}	↘	3.572	3.547	3.350	3.293
$\varepsilon_{1(MIT)}$	↘	12.76	12.58	11.21	10.84
R_{MIT}	↘	0.316	0.314	0.292	0.285
At **x=1**,					
E_{CPE} in meV	↗	810	810.1	811.5	812
n_{MIT}	↘	4.050	4.023	3.810	3.750
$\varepsilon_{1(MIT)}$	↘	16.40	16.19	14.52	14.06
R_{MIT}	↘	0.365	0.362	0.341	0.335

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	↗	1281.5	1303	1309	1312
n_{MIT}	↘	4.340	3.572	3.477	3.434
$\varepsilon_{1(MIT)}$	↘	18.83	12.76	12.09	11.79
R_{MIT}	↘	0.391	0.316	0.306	0.301
At **x=1**,					

E_{CPE} in meV	↗	798.2	810	813	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, at T=0K and N=$N_{CDn(p)}(r_{d(a)},x)$, and as $E \to \infty$, the numerical results of $n_\infty(r_{d(a)},x)$, $\varepsilon_{1,\infty}(r_{d(a)},x)$, $\sigma_{O,\infty}(r_{d(a)},x)$, $\alpha_\infty(r_{d(a)},x)$ and $R_\infty(r_{d(a)},x)$ go to their appropriate limiting constants.

Donor		P	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
$\sigma_{O,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	8.638	8.535	7.721	7.491
$\propto_\infty$ in $(10^9 \times cm^{-1}) = 2.1602$					
R_∞	↘	0.095	0.092	0.066	0.059
At **x=0.5**,					
n_∞	↘	2.080	2.055	1.860	1.803
$\varepsilon_{1,\infty}$	↘	4.325	4.222	3.455	3.252
$\sigma_{O,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	9.489	9.376	8.482	8.229
$\propto_\infty$ in $(10^9 \times cm^{-1}) = 2.1602$					
R_∞	↘	0.123	0.119	0.090	0.082
At **x=1**,					
n_∞	↘	2.251	2.224	2.012	1.952
$\varepsilon_{1,\infty}$	↘	5.066	4.945	4.047	3.810
$\sigma_{O,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	10.270	10.147	9.180	8.906
$\propto_\infty$ in $(10^9 \times cm^{-1}) = 2.1602$					
R_∞	↘	0.148	0.144	0.113	0.104

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
$\sigma_{O,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	11.77	8.64	8.26	8.09
$\propto_\infty$ in $(10^9 \times cm^{-1}) = 2.1602$					
R_∞	↘	0.195	0.095	0.083	0.078
At **x=0.5**,					
n_∞	↘	2.834	2.080	1.988	1.948

$\varepsilon_{1,\infty}$	↘	8.031	4.325	3.952	3.794
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	12.93	9.489	9.071	8.888
$\propto_{\infty}$ in $(10^9 \times cm^{-1}) = 2.1602$					
R_{∞}	↘	0.229	0.123	0.109	0.103
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 $(10^9 \times cm^{-1}) = 2.1602$					
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,				
$\mathbf{E_{CPE} = 1.796}$	**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,				
$\mathbf{E_{CPE}}$ **=1.3030**	**3.5720**	**0**	**12.7594**	**0**
2	4.189	0.212	17.507	1.780
2.5	4.988	0.542	24.589	5.412
3	4.841	2.365	17.840	22.903
3.5	3.716	2.513	7.495	18.682
4	3.880	2.202	10.206	17.085
4.5	4.285	3.326	7.300	28.504
5	2.283	4.569	−15.662	20.862
5.5	0.946	3.186	−9.256	6.026

6	1.115	2.352	−4.287	5.246
…				
10^{22}	**2.0796**	**0**	**4.3248**	**0**
At x=1,				
E_{CPE} =0.81	**4.0503**	**0**	**16.4053**	**0**
2	5.326	0.136	28.346	1.449
2.5	6.440	1.081	40.302	13.926
3	5.767	3.940	17.742	45.443
3.5	3.891	3.768	0.941	29.320
4	4.118	3.080	7.467	25.366
4.5	4.646	4.431	1.950	41.168
5	2.046	5.868	−30.252	24.020
5.5	0.427	3.978	−15.645	3.401
6	0.711	2.871	−7.739	4.085
…				
10^{22}	**2.2507**	**0**	**5.0658**	**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	9.896
6	2.040	1.919	0.477	7.830
…				
10^{22}	**2.5797**	**0**	**6.6548**	**0**
At x=0.5,				
E_{CPE} =1.2815	**4.3397**	**0**	**18.8329**	**0**
2	4.982	0.210	24.777	2.096
2.5	5.794	0.562	33.251	6.514

3	5.627	2.426	25.784	27.304
3.5	4.473	2.563	13.443	22.930
4	4.640	2.237	16.516	20.755
4.5	5.049	3.371	14.128	34.038
5	3.022	4.622	−12.231	27.938
5.5	1.673	3.219	−7.562	10.769
6	1.847	2.373	−2.222	8.767
…				
10^{22}	**2.8339**	**0**	**8.0308**	**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 $\mathbf{r_d}$ 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 $\mathbf{r_d} = \mathbf{r_P}$,					
$\eta_n \gg 1$	↗	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 $\mathbf{r_d} = \mathbf{r_P}$,

$\eta_n \gg 1$	↗	177	256	447	629
E_{gn1} in eV	↗	1.154	1.148	1.197	1.273
n	↘	4.565	4.562	4.520	4.452
κ	↘	3.130	3.120	2.975	2.752
ε_1	↗	11.045	11.080	11.580	12.249
ε_2	↘	28.577	28.474	26.897	24.505

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

$\eta_n \gg 1$	↗	177	255.8	447	628.6
E_{gn1} in eV	↗	1.216	1.242	1.339	1.458
n	↘	4.282	4.259	4.172	4.063
κ	↘	2.917	2.842	2.567	2.250
ε_1	↗	9.828	10.064	10.817	11.447
ε_2	↘	24.981	24.212	21.419	18.290

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

$\eta_n \gg 1$	↗	176.9	255.7	447	628.5
E_{gn1} in eV	↗	1.233	1.264	1.372	1.500
n	↘	4.212	4.184	4.086	3.968
κ	↘	2.868	2.779	2.476	2.141
ε_1	↗	9.514	9.787	10.568	11.161

ε_2	↘	24.161	23.258	20.238	16.992
x=1					
For $\mathbf{r_d} = \mathbf{r_P}$,					
$\eta_n \gg 1$	↗	316.5	456.8	797.7	1121.4
E_{gn1} in eV	↗	0.601	0.671	0.808	0.985
n	↘	5.152	5.129	5.020	4.873
κ	↘	4.855	4.740	4.242	3.636
ε_1	↗	2.978	3.835	7.205	10.526
ε_2	↘	50.029	48.619	42.585	35.444
For $\mathbf{r_d} = \mathbf{r_{Sb}}$,					
$\eta_n \gg 1$	↗	316.5	456.8	797.7	1121.4
E_{gn1} in eV	↗	0.759	0.827	1.046	1.294
n	↘	4.820	4.765	4.583	4.366
κ	↘	4.418	4.173	3.438	2.693
ε_1	↗	3.721	5.291	9.179	11.808
ε_2	↘	42.589	39.772	31.513	23.513
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↗	316.5	456.7	797.7	1121.4
E_{gn1} in eV	↗	0.786	0.863	1.102	1.366
n	↘	4.738	4.676	4.475	4.241
κ	↘	4.319	4.047	3.264	2.494
ε_1	↗	3.797	5.484	9.375	11.765
ε_2	↘	40.933	37.844	29.213	21.155
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 $\mathbf{r_a} = \mathbf{r_{Ga}}$,					
$\eta_p \gg 1$	↗	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 $\mathbf{r_a} = \mathbf{r_{Ga}}$,					
$\eta_p \gg 1$	↗	154.7	237.4	433.3	617
E_{gp1} in eV	↗	1.134	1.137	1.196	1.285
n	↘	4.575	4.572	4.521	4.441
κ	↘	3.165	3.154	2.977	2.717
ε_1	↗	10.916	10.9575	11.574	12.341
ε_2	↘	28.960	28.838	26.916	24.138
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↗	147.3	231.5	428.9	613.4
E_{gp1} in eV	↗	1.161	1.172	1.248	1.353
n	↘	4.460	4.450	4.383	4.289
κ	↘	3.082	3.049	2.824	2.529
ε_1	↗	10.3914	10.5098	11.236	11.998
ε_2	↘	27.492	27.135	24.753	21.692

For $\mathbf{r_a} = \mathbf{r_{Cd}}$,					
$\eta_p \gg 1$	↗	147.1	228.2	426.5	611.3
E_{gp1} in eV	↗	1.172	1.187	1.270	1.382
n	↘	4.409	4.397	4.323	4.222
κ	↘	3.047	3.005	2.760	2.451
ε_1	↗	10.1573	10.3045	11.068	11.820
ε_2	↘	26.875	26.427	23.866	20.700
		x=1			
For $\mathbf{r_a} = \mathbf{r_{Ga}}$,					
$\eta_p \gg 1$	↗	306.2	448.2	791.2	1115.9
E_{gp1} in eV	↗	0.582	0.607	0.741	0.919
n	↘	5.198	5.178	5.074	4.928
κ	↘	5.080	4.982	4.484	3.856
ε_1	↗	1.206	1.991	5.639	9.423
ε_2	↘	52.817	51.601	45.499	38.005
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↗	302.9	445.5	789.2	1114.2
E_{gp1} in eV	↗	0.628	0.668	0.833	1.039
n	↘	5.063	5.032	4.900	4.729
κ	↘	4.905	4.753	4.154	3.462
ε_1	↗	1.581	2.728	6.760	10.376
ε_2	↘	49.673	47.843	40.711	32.740
For $\mathbf{r_a} = \mathbf{r_{Cd}}$,					
$\eta_p \gg 1$	↗	301.1	444.0	788.1	1113.3
E_{gp1} in eV	↗	0.647	0.693	0.872	1.090
n	↘	5.005	4.969	4.825	4.642
κ	↘	4.832	4.658	4.018	3.301
ε_1	↗	1.703	2.986	7.136	10.647
ε_2	↘	48.366	46.293	38.772	30.647
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 $\mathbf{r_d = r_P}$,					
$\eta_n \gg 1$	↘	628.7	251.5	127.7	41.9
E_{gn1} in eV	↘	1.273	1.266	1.247	1.144
n	↗	4.452	4.459	4.475	4.566
κ	↗	2.752	2.772	2.826	3.134
ε_1	↘	12.249	12.192	12.040	11.031

ε_2	↗	24.505	24.724	25.295	28.620

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

$\eta_n \gg 1$	↘	628.6	251.4	125.7	41.88
E_{gn1} in eV	↘	1.458	1.450	1.432	1.328
n	↗	4.063	4.070	4.087	4.182
κ	↗	2.250	2.269	2.318	2.597
ε_1	↘	11.447	11.417	11.335	10.744
ε_2	↗	18.290	18.472	18.946	21.721

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

$\eta_n \gg 1$	↘	628.5	251.4	125.7	41.88
E_{gn1} in eV	↘	1.500	1.493	1.475	1.371
n	↗	3.968	3.975	3.992	4.087
κ	↗	2.141	2.159	2.206	2.479
ε_1	↘	11.161	11.137	11.068	10.561
ε_2	↗	16.992	17.165	17.618	20.269

x=1

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

$\eta_n \gg 1$	↘	1121.4	448.6	224.3	74.7
E_{gn1} in eV	↘	0.985	0.981	0.968	0.889
n	↗	4.873	4.877	4.887	4.953
κ	↗	3.636	3.651	3.692	3.958
ε_1	↘	10.526	10.458	10.258	8.869
ε_2	↗	35.444	35.610	36.090	39.210

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

$\eta_n \gg 1$	↘	1121.4	448.5	224.3	74.7
E_{gn1} in eV	↘	1.294	1.290	1.277	1.198
n	↗	4.366	4.370	4.381	4.451
κ	↗	2.693	2.705	2.741	2.970
ε_1	↘	11.808	11.776	11.681	10.988
ε_2	↗	23.513	23.642	24.014	26.444

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

$\eta_n \gg 1$	↘	1121.4	448.5	224.3	74.7
E_{gn1} in eV	↘	1.366	1.361	1.349	1.270
n	↗	4.241	4.245	4.256	4.327

κ	↗	2.494	2.506	2.540	2.761
ε_1	↘	11.765	11.739	11.663	11.101
ε_2	↗	21.155	21.275	21.623	23.901
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 $\mathbf{r_a = r_{Ga}}$,					

$\eta_p \gg 1$	↘	617	247	123	41
E_{gp1} in eV	↘	1.285	1.278	1.260	1.156
n	↗	4.441	4.448	4.464	4.556
κ	↗	2.717	2.738	2.791	3.097
ε_1	↘	12.341	12.287	12.141	11.164
ε_2	↗	24.138	24.354	24.920	28.217
For $\mathbf{r_a = r_{In}}$,					
$\eta_p \gg 1$	↘	613	245	122.7	40.87
E_{gp1} in eV	↘	1.353	1.346	1.327	1.224
n	↗	4.289	4.295	4.312	4.405
κ	↗	2.529	2.549	2.600	2.895
ε_1	↘	11.998	11.954	11.834	11.018
ε_2	↗	21.692	21.894	22.423	25.508
For $\mathbf{r_a = r_{Cd}}$,					
$\eta_p \gg 1$	↘	611	244.5	122.3	40.73
E_{gp1} in eV	↘	1.382	1.374	1.356	1.252
n	↗	4.222	4.229	4.246	4.339
κ	↗	2.451	2.470	2.521	2.812
ε_1	↘	11.820	11.780	11.671	10.919
ε_2	↗	20.700	20.896	21.409	24.405
			x=1		
For $\mathbf{r_a = r_{Ga}}$,					
$\eta_p \gg 1$	↘	1115.9	446	223	74
E_{gp1} in eV	↘	0.919	0.915	0.902	0.823
n	↗	4.928	4.932	4.942	5.007
κ	↗	3.856	3.870	3.913	4.186
ε_1	↘	9.423	9.344	9.116	7.544
ε_2	↗	38.005	38.178	38.678	41.925
For $\mathbf{r_a = r_{In}}$,					
$\eta_p \gg 1$	↘	1114.2	445.7	222.8	74.3
E_{gp1} in eV	↘	1.039	1.035	1.022	0.943
n	↗	4.729	4.732	4.743	4.809
κ	↗	3.462	3.476	3.516	3.776
ε_1	↘	10.376	10.314	10.134	8.875

ε_2	↗	32.740	32.899	33.354	36.319
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For $\mathbf{r_a} = \mathbf{r_{Cd}}$,					
$\eta_p \gg 1$	↘	1113.3	445.3	222.6	74.2
E_{gp1} in eV	↘	1.090	1.085	1.073	0.994
n	↗	4.642	4.645	4.656	4.723
κ	↗	3.301	3.315	3.354	3.608
ε_1	↘	10.647	10.591	10.429	9.293
ε_2	↗	30.647	30.799	31.235	34.083
T in K	↗	20	50	100	300