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OPTICAL COEFFICIENTS IN THE N(P)-TYPE DEGENERATE GaP(1-x) As(x)-CRYSTALLINE ALLOY, DUE TO THE NEW STATIC DIELECTRIC CONSTANT-LAW AND THE GENERALIZED MOTT CRITERIUM IN THE METAL-INSULATOR TRANSITION (16)

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ABTRACT

In the n(p)-type $\mathbf{GaP_{1-x}As_x}$- crystalline alloy, with $0 \leq x \leq 1$, basing on our two recent works[1,2], for a given x, and with an increasing $r_{d(a)}$, the optical coefficients have been determined, as functions of the photon energy E, total impurity density N, the donor (acceptor) radius $r_{d(a)}$, concentration x, and temperature T. Those results have been affected by **(i)** the important new $\varepsilon(r_{d(a)}, x)$ -law, developed in Equations (8a, 8b), stating that, for a given x, due to the impurity-size effect, ε decreases (↘) with an increasing (↗) $r_{d(a)}$, and then by **(ii)** the generalized Mott critical d(a)-density defined in the metal-insulator transition (MIT), $N_{CDn(NDp)}(r_{d(a)}, x)$, as observed in Equations (8c, 9a). Furthermore, we also showed that $N_{CDn(NDp)}$ is just the density of carriers localized in exponential band tails, with a precision of the order of $\mathbf{2.92 \times 10^{-7}}$, 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: $GaP_{1-x}As_x$ - crystalline alloy; impurity-size effect; Mott critical impurity density in the MIT, optical coefficients.

INTRODUCTION

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

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

ENERGY BAND STUCTURE PARAMETERS

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

$$m_{c(v)}(x)/m_o = 0.066\ (0.291) \times x + 0.13(0.5) \times (1 - x) \quad (1)$$

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

$$\varepsilon_o(x) = 13.13 \times x + 11.1 \times (1 - x). \quad (2)$$

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

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

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

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

and then, the isothermal bulk modulus, by:

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

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:

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

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

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

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

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

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

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

$$a_{Bn(Bp)}(r_{d(a)},x) \equiv \frac{\varepsilon(r_{d(a)},x)\times\hbar^2}{m_{c(v)}(x)\times q^2} = 0.53\times10^{-8}\ \text{cm} \times \frac{\varepsilon(r_{d(a)},x)}{m_{c(v)}(x)/m_o}. \quad (8c)$$

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:

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

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

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

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 $\boldsymbol{\mathcal{H}_{n(p)}} = \mathbf{0.47137}$, 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:

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

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:

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

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 $r_{d(a)}$

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

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

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

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

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

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

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

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

$$\Delta E_{gno}(N, r_d, x) \simeq a_1 \times \frac{\varepsilon_0(x)}{\varepsilon(r_d,x)} \times N_r^{1/3} + a_2 \times \frac{\varepsilon_0(x)}{\varepsilon(r_d,x)} \times N_r^{\frac{1}{3}} \times (2.503 \times [-E_{cn}(r_{sn}) \times r_{sn}]) + a_3 \times \left[\frac{\varepsilon_0(x)}{\varepsilon(r_d,x)}\right]^{5/4} \times \sqrt{\frac{m_v}{m_r}} \times N_r^{1/4} + a_4 \times \sqrt{\frac{\varepsilon_0(x)}{\varepsilon(r_d,x)}} \times N_r^{1/2} \times 2 + a_5 \times \left[\frac{\varepsilon_0(x)}{\varepsilon(r_d,x)}\right]^{\frac{3}{2}} \times N_r^{\frac{1}{6}},$$

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

$$\Delta E_{gn}(N, r_d, x) = \Delta E_{gno}(N, r_d, x) \times \{1.3 \times x + 2.2 \times (1 - x)\}, \quad (14n)$$

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:

$$\Delta E_{gpo}(N, r_a, x) \simeq a_1 \times \frac{\varepsilon_0(x)}{\varepsilon(r_a,x)} \times N_r^{1/3} + a_2 \times \frac{\varepsilon_0(x)}{\varepsilon(r_a,x)} \times N_r^{\frac{1}{3}} \times \left(2.503 \times [-E_{cp}(r_{sp}) \times r_{sp}]\right) + a_3 \times \left[\frac{\varepsilon_0(x)}{\varepsilon(r_a,x)}\right]^{5/4} \times \sqrt{\frac{m_c}{m_r}} \times N_r^{1/4} + 2a_4 \times \sqrt{\frac{\varepsilon_0(x)}{\varepsilon(r_a,x)}} \times N_r^{1/2} + a_5 \times \left[\frac{\varepsilon_0(x)}{\varepsilon(r_a,x)}\right]^{\frac{3}{2}} \times N_r^{\frac{1}{6}},$$

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

$$\Delta E_{gp}(N, r_a, x) = \Delta E_{gpo}(N, r_a, x) \times \{13 \times x + 18 \times (1 - x)\}, \quad (14p)$$

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:

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

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]

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

$\varepsilon_1 \equiv n^2 - \kappa^2$ and $\varepsilon_2 \equiv 2n\kappa$, (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 $E \gtrsim E_{gn1(gp1)}$,

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

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 $E\rightarrow\infty$, Forouhi and Bloomer (FB)[4] claimed that $\kappa(E\rightarrow\infty)\rightarrow$ 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:

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

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

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

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

going to a constant as $E\rightarrow\infty$, since $n(E\rightarrow\infty,r_{d(a)},x)\rightarrow n_\infty(r_{d(a)},x)=\sqrt{\varepsilon(r_{d(a)},x)}\times\frac{\omega_T}{\omega_L}$, $\omega_T=5.1\times10^{13}\ s^{-1}$ [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, $\mathbf{n}$ and $\boldsymbol{\kappa}$, 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 $(\mathbf{x}) \equiv \mathbf{GaP_{1-x}As_x}$- crystalline alloy, as follows.

A. Metal-insulator transition (MIT)-case

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

Then, in this MIT-case, if $E = E_{gn1(gp1)}(r_{d(a)}, x) = E_{gno(gpo)}(r_{d(a)}, x)$, which can be defined as the critical photon energy: $E \equiv E_{CPE}(r_{d(a)}, x)$, one obtains: $\kappa_{MIT}(r_{d(a)}, x) = 0$ from Eq. (20), and from Eq. (16): $\varepsilon_{2(MIT)}(r_{d(a)}, x) = 0$, $\sigma_{O(MIT)}(r_{d(a)}, x) = 0$ and $\propto_{MIT}(r_{d(a)}, x) = 0$, 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 $N = 10^{20}\text{cm}^{-3}$, 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 $\mathbf{X(x) \equiv GaP_{1-x}As_x}$- crystalline alloy, by basing on our two recent works[1,2], for a given x, and with an increasing $r_{d(a)}$, the optical coefficients have been determined, as functions of the photon energy E, total impurity density N, the donor (acceptor) radius $r_{d(a)}$, concentration x, and temperature T.

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

Further, we also showed that $N_{CDn(NDp)}$ is just the density of carriers localized in exponential band tails, with a precision of the order of $\mathbf{2.92 \times 10^{-7}}$, 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	↗	1658	1658.4	1663	1665
n_{MIT}	↘	3.249	3.225	3.036	2.982
$\varepsilon_{1(MIT)}$	↘	10.55	10.40	9.22	8.89
R_{MIT}	↘	0.280	0.277	0.254	0.248
At **x=1**,					
E_{CPE} in meV	↗	1520	1520.2	1522.9	1524
n_{MIT}	↘	3.416	3.391	3.196	3.140
$\varepsilon_{1(MIT)}$	↘	11.67	11.50	10.21	9.86
R_{MIT}	↘	0.299	0.296	0.274	0.267
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	↗	1631.98	1658	1665	1669
n_{MIT}	↘	3.982	3.249	3.157	3.117
$\varepsilon_{1(MIT)}$	↘	15.86	10.55	9.97	9.71
R_{MIT}	↘	0.358	0.280	0.269	0.264
At **x=1**,					

E_{CPE} in meV	↗	1503.7	1520	1524	1527
n_{MIT}	↘	4.173	3.416	3.323	3.281
$\varepsilon_{1(MIT)}$	↘	17.41	11.67	11.04	10.77
R_{MIT}	↘	0.376	0.299	0.289	0.284

Table 2. Here, 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
α_∞ in $(10^9 \times cm^{-1}) = 2.1602$					
R_∞	↘	0.095	0.092	0.066	0.059
At **x=0.5**,					
n_∞	↘	1.978	1.954	1.768	1.715
$\varepsilon_{1,\infty}$	↘	3.911	3.818	3.125	2.942
$\sigma_{O,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	9.025	8.916	8.067	7.826
α_∞ in $(10^9 \times cm^{-1}) = 2.1602$					
R_∞	↘	0.108	0.104	0.077	0.069
At **x=1**,					
n_∞	↘	2.059	2.034	1.840	1.785
$\varepsilon_{1,\infty}$	↘	4.239	4.138	3.387	3.188
$\sigma_{O,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	9.395	9.282	8.398	8.147
α_∞ in $(10^9 \times cm^{-1}) = 2.1602$					
R_∞	↘	0.120	0.116	0.087	0.079
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
α_∞ in $(10^9 \times cm^{-1}) = 2.1602$					
R_∞	↘	0.195	0.095	0.083	0.078
At **x=0.5**,					
n_∞	↘	2.695	1.978	1.891	1.852

$\varepsilon_{1,\infty}$ ↘	7.263	3.911	3.575	3.431
$\sigma_{O,\infty}$ in $\frac{10^5}{\Omega \times cm}$ ↘	12.30	9.025	8.627	8.452
α_∞ in $(10^9 \times cm^{-1}) = 2.1602$				
R_∞ ↘	0.210	0.108	0.095	0.089
At **x=1**,				
n_∞ ↘	2.806	2.059	1.968	1.928
$\varepsilon_{1,\infty}$ ↘	7.872	4.239	3.874	3.718
$\sigma_{O,\infty}$ in $\frac{10^5}{\Omega \times cm}$ ↘	12.80	9.39	8.981	8.799
α_∞ in $(10^9 \times cm^{-1}) = 2.1602$				
R_∞ ↘	0.225	0.120	0.106	0.100

Table 3n. In the P-X(x)-system, and at T=0K and $N = N_{CDn}(r_p, x)$, according to the MIT, our numerical results of n, κ, ε_1 and ε_2 are obtained from Equations (21, 20, 16), respectively, and expressed as functions of $E\ [\geq E_{CPE}(r_p, x)]$ and x, noting that (i) $\kappa = 0$ and $\varepsilon_2 = 0$ at $E = E_{CPE}(r_p, x)$, and $\kappa \to 0$ and $\varepsilon_2 \to 0$ as $E \to \infty$.

E in eV	n	κ	ε_1	ε_2
At x=0,				
$E_{CPE} = 1.796$	**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
…				
10^{22}	**1.8931**	**0**	**3.5838**	**0**
At x=0.5,				
E_{CPE} =1.6580	**3.2489**	**0**	**10.5557**	**0**
2	3.506	0.213	12.248	1.498
2.5	4.105	0.268	16.782	2.204
3	4.217	1.479	15.599	12.478
3.5	3.536	1.767	9.382	12.494
4	3.673	1.660	10.736	12.197
4.5	4.009	2.628	9.165	21.074
5	2.396	3.733	−8.200	17.888
5.5	1.251	2.670	−5.564	6.678

6	1.354	2.010	−2.206	5.442
…				
10^{22}	**1.9777**	**0**	**3.9115**	**0**
At x=1,				
E_{CPE} =1.658	**3.2489**	**0**	**10.5557**	**0**
2	3.506	0.213	12.248	1.498
2.5	4.105	0.268	16.782	2.204
3	4.217	1.479	15.599	12.478
3.5	3.536	1.767	9.382	12.494
4	3.673	1.660	10.736	12.197
4.5	4.009	2.628	9.165	21.074
5	2.396	3.733	−8.200	17.888
5.5	1.251	2.670	−5.564	6.678
6	1.354	2.010	−2.206	5.442
…				
10^{22}	**1.9777**	**0**	**3.9115**	**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} =1.6320	**3.9825**	**0**	**15.8601**	**0**
2	4.263	0.216	18.125	1.845
2.5	4.876	0.285	23.693	2.782

3	4.972	1.537	22.362	15.288
3.5	4.261	1.817	14.856	15.485
4	4.400	1.697	16.477	14.936
4.5	4.740	2.677	15.305	25.376
5	3.099	3.792	−4.771	23.505
5.5	1.941	2.706	−3.557	10.503
6	2.048	2.034	0.059	8.333
…				
10^{22}	**2.6951**	**0**	**7.2634**	**0**
At x=1,				
E_{CPE} =1.5037	**4.1730**	**0**	**17.4142**	**0**
2	4.575	0.222	20.883	2.033
2.5	5.258	0.376	27.589	3.952
3	5.270	1.839	24.390	19.384
3.5	4.406	2.075	15.106	18.286
4	4.552	1.886	17.168	17.174
4.5	4.916	2.921	15.638	28.727
5	3.138	4.086	−6.847	25.649
5.5	1.911	2.888	−4.692	11.040
6	2.041	2.155	−0.477	8.999
…				
10^{22}	**2.8057**	**0**	**7.8719**	**0**

E in eV	n	κ	ε_1	ε_2

Table 4n. In the X(x)-system, at E=3.2 eV and T=20 K, for given r_d and x, and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of $\eta_n (\gg 1, \text{degenerate case})$, E_{gn1}, n, κ, ε_1 and ε_2, obtained as functions of N, being represented by the arrows: ↗ and ↘, noting that both η_n and E_{gn1} increase with increasing N.

N (10^{18} cm^{-3}) ↗	15	26	60	100
		x=0		
For $\mathbf{r_d = r_P}$,				
$\eta_n \gg 1$ ↗	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 $\mathbf{r_d = r_{Sb}}$,				

$\eta_n \gg 1$	↗	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 $r_d = r_{Sn}$,

$\eta_n \gg 1$	↗	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

x=0.5

For $r_d = r_P$,

$\eta_n \gg 1$	↗	163	236	412	580
E_{gn1} in eV	↗	1.524	1.532	1.587	1.666
n	↘	4.120	4.113	4.061	3.985
κ	↘	2.081	2.062	1.929	1.743
ε_1	↗	12.642	12.661	12.769	12.837
ε_2	↘	17.148	16.966	15.669	13.895

For $r_d = r_{Sb}$,

$\eta_n \gg 1$	↗	163	236	412	580
E_{gn1} in eV	↗	1.588	1.615	1.712	1.828
n	↘	3.850	3.824	3.730	3.616
κ	↘	1.927	1.863	1.641	1.394
ε_1	↗	11.110	11.155	11.222	↘ 11.129
ε_2	↘	14.838	14.248	12.240	10.085

For $r_d = r_{Sn}$,

$\eta_n \gg 1$	↗	163	235.5	412	580
E_{gn1} in eV	↗	1.603	1.634	1.742	1.866
n	↘	3.783	3.753	3.649	3.525
κ	↘	1.891	1.817	1.576	1.319
ε_1	↗	10.735	10.782	10.828	↘ 10.688
ε_2	↘	14.311	13.640	11.505	9.297

		x=1			
For $\mathbf{r_d = r_P}$,					
$\eta_n \gg 1$	↗	239	345	602	847
E_{gn1} in eV	↗	1.338	1.348	1.425	1.537
n	↘	4.373	4.364	4.294	4.200
κ	↘	2.569	2.541	2.335	2.049
ε_1	↗	12.522	12.584	12.981	13.348
ε_2	↘	22.470	22.181	20.055	17.169
For $\mathbf{r_d = r_{Sb}}$,					
$\eta_n \gg 1$	↗	239	345	602	847
E_{gn1} in eV	↗	1.432	1.473	1.615	1.783
n	↘	4.068	4.031	3.897	3.733
κ	↘	2.316	2.212	1.863	1.489
ε_1	↗	11.187	11.357	11.715	11.722
ε_2	↘	18.844	17.831	14.520	11.117
For $\mathbf{r_d = r_{Sn}}$,					
$\eta_n \gg 1$	↗	239	345	602	847
E_{gn1} in eV	↗	1.454	1.502	1.659	1.840
n	↘	3.993	3.949	3.800	3.622
κ	↘	2.259	2.138	1.761	1.371
ε_1	↗	10.843	11.023	11.337	↘ 11.238
ε_2	↘	18.039	16.889	13.382	9.934
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 $\mathbf{r_a = r_{In}}$,

$\eta_p \gg 1$	↗	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 $\mathbf{r_a = r_{Cd}}$,

$\eta_p \gg 1$	↗	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

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x=0.5

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

$\eta_p \gg 1$	↗	135	214	396	566
E_{gp1} in eV	↗	1.537	1.552	1.631	1.734
n	↘	4.108	4.094	4.019	3.918
κ	↘	2.049	2.013	1.825	1.592
ε_1	↗	12.6741	12.7071	12.8196	↘ 12.8189
ε_2	↘	16.838	16.483	14.665	12.477

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

$\eta_p \gg 1$	↗	127	206	390	561
E_{gp1} in eV	↗	1.560	1.581	1.674	1.790
n	↘	3.999	3.980	3.890	3.776
κ	↘	1.994	1.944	1.726	1.473
ε_1	↗	12.0185	12.059	12.153	↘ 12.0908
ε_2	↘	15.953	15.474	13.426	11.125

For $\mathbf{r_a = r_{Cd}}$,					
$\eta_p \gg 1$	↗	121	202	387	559
E_{gp1} in eV	↗	1.569	1.592	1.692	1.814
n	↘	3.952	3.930	3.834	3.714
κ	↘	1.971	1.915	1.685	1.424
ε_1	↗	11.7334	11.776	11.861 ↘	11.770
ε_2	↘	15.583	15.057	12.920	10.579
		x=1			
For $\mathbf{r_a = r_{Ga}}$,					
$\eta_p \gg 1$	↗	227	335	595	840
E_{gp1} in eV	↗	1.377	1.406	1.529	1.684
n	↘	4.338	4.311	4.196	4.049
κ	↘	2.464	2.385	2.096	1.704
ε_1	↗	12.746	12.895	13.330	13.490
ε_2	↘	21.375	20.565	17.365	13.800
For $\mathbf{r_a = r_{In}}$,					
$\eta_p \gg 1$	↗	223	332	592	838
E_{gp1} in eV	↗	1.409	1.449	1.594	1.767
n	↘	4.217	4.181	4.044	3.876
κ	↘	2.377	2.273	1.912	1.521
ε_1	↗	12.137	12.313	12.703	12.713
ε_2	↘	20.049	19.011	15.465	11.793
For $\mathbf{r_a = r_{Cd}}$,					
$\eta_p \gg 1$	↗	221	330	592	837
E_{gp1} in eV	↗	1.423	1.467	1.621	1.803
n	↘	4.165	4.124	3.978	3.801
κ	↘	2.341	2.227	1.847	1.446
ε_1	↗	11.868	12.052	12.416 ↘	12.358
ε_2	↘	19.498	18.371	14.696	10.997
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 $r_d = r_p$,					
$\eta_n \gg 1$	↘	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 $r_d = r_{Sb}$,					
$\eta_n \gg 1$	↘	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 $r_d = r_{Sn}$,					
$\eta_n \gg 1$	↘	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 $r_d = r_p$,					
$\eta_n \gg 1$	↘	580	232	116	38.6
E_{gn1} in eV	↘	1.666	1.659	1.641	1.537
n	↗	3.985	3.991	4.009	4.108
κ	↗	1.743	1.760	1.803	2.050
ε_1	↘	12.837	12.835	12.826	12.673

ε_2	↗	13.895	14.050	14.456	16.844

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

$\eta_n \gg 1$	↘	579.8	231.9	115.9	38.6
E_{gn1} in eV	↘	1.828	1.821	1.803	1.699
n	↗	3.616	3.623	3.641	3.743
κ	↗	1.394	1.409	1.447	1.670
ε_1	↗	11.129	11.139	11.164	11.221
ε_2	↗	10.085	10.211	10.542	12.502

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

$\eta_n \gg 1$	↘	579.7	231.9	115.9	38.6
E_{gn1} in eV	↘	1.866	1.859	1.840	1.737
n	↗	3.525	3.532	3.551	3.653
κ	↗	1.319	1.333	1.370	1.587
ε_1	↗	10.688	10.701	10.732	10.829
ε_2	↗	9.297	9.417	9.731	11.595

x=1

For $\mathbf{r_d = r_P}$,

$\eta_n \gg 1$	↘	847	338.8	169	56
E_{gn1} in eV	↘	1.537	1.533	1.520	1.441
n	↗	4.189	4.193	4.205	4.278
κ	↗	2.049	2.060	2.091	2.293
ε_1	↘	13.348	13.338	13.308	13.050
ε_2	↗	17.169	17.276	17.585	19.618

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

$\eta_n \gg 1$	↘	846.9	338.7	169	56
E_{gn1} in eV	↘	1.738	1.734	1.721	1.642
n	↗	3.722	3.727	3.739	3.815
κ	↗	1.584	1.593	1.621	1.799
ε_1	↗	11.348	11.350	11.353 ↘	11.323
ε_2	↗	11.792	11.876	12.119	13.726

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

$\eta_n \gg 1$	↘	846.8	338.7	169	56
E_{gn1} in eV	↘	1.840	1.835	1.823	1.744
n	↗	3.622	3.626	3.639	3.717

κ	↗	1.371	1.380	1.405	1.571
ε_1	↗	11.238	11.246	11.265	11.345
ε_2	↗	9.934	10.010	10.229	11.683
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 $r_a = r_{Ga}$,					
$\eta_p \gg 1$	↘	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 $r_a = r_{In}$,					
$\eta_p \gg 1$	↘	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 $r_a = r_{Cd}$,					
$\eta_p \gg 1$	↘	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 $r_a = r_{Ga}$,					
$\eta_p \gg 1$	↘	566	226	113	38

E_{gp1} in eV	↘	1.734	1.727	1.709	1.605
n	↗	3.918	3.925	3.943	4.043
κ	↗	1.592	1.608	1.648	1.885
ε_1	↗	12.819	12.824	12.834 ↘	12.794
ε_2	↗	12.477	12.622	13.002	15.248

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

$\eta_p \gg 1$	↘	561	225	112	37
E_{gp1} in eV	↘	1.790	1.783	1.765	1.661
n	↗	3.776	3.783	3.802	3.903
κ	↗	1.473	1.488	1.527	1.756
ε_1	↗	12.091	12.099	12.120	12.148
ε_2	↗	11.125	11.259	11.613	13.704

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

$\eta_p \gg 1$	↘	559	224	112	37
E_{gp1} in eV	↘	1.814	1.807	1.788	1.685
n	↗	3.714	3.722	3.740	3.841
κ	↗	1.424	1.439	1.477	1.702
ε_1	↗	11.770	11.781	11.805	11.859
ε_2	↗	10.579	10.709	11.051	13.078

x=1

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

$\eta_p \gg 1$	↘	840	336	168	56
E_{gp1} in eV	↘	1.684	1.679	1.667	1.588
n	↗	4.049	4.053	4.065	4.141
κ	↗	1.704	1.714	1.742	1.927
ε_1	↗	13.490	13.4905	13.4908 ↘	13.437
ε_2	↗	13.800	13.894	14.165	15.957

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

$\eta_p \gg 1$	↘	838	335	168	56
E_{gp1} in eV	↘	1.767	1.763	1.751	1.672
n	↗	3.876	3.881	3.893	3.970
κ	↗	1.521	1.530	1.557	1.732
ε_1	↗	12.713	12.7181	12.731	12.763
ε_2	↗	11.793	11.878	12.123	13.749

For $\mathbf{r_a = r_{Cd}}$,					
$\eta_p \gg 1$	↘	837	335	167	56
E_{gp1} in eV	↘	1.803	1.799	1.786	1.707
n	↗	3.801	3.806	3.818	3.896
κ	↗	1.446	1.455	1.481	1.652
ε_1	↗	12.358	12.3649	12.383	12.447
ε_2	↗	10.997	11.078	11.314	12.871
T in K	↗	20	50	100	300