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OPTICAL COEFFICIENTS IN THE N(P)-TYPE DEGENERATE Si(1-x) Ge(x)-CRYSTALLINE ALLOY, DUE TO THE NEW STATIC DIELECTRIC CONSTANT-LAW AND THE GENERALIZED MOTT CRITERIUM IN THE METAL-INSULATOR TRANSITION (19)

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ABTRACT:

In the n(p)-type $\mathbf{Si_{1-x}Ge_x}$- crystalline alloy, with $0 \leq x \leq 1$, basing on our two recent works[1,2], for a given x, and with an increasing $r_{d(a)}$, the optical coefficients have been determined, as functions of the photon energy E, total impurity density N, the donor (acceptor) radius $r_{d(a)}$, concentration x, and temperature T. Those results have been affected by **(i)** the important new $\varepsilon(r_{d(a)}, x)$ -law, developed in Equations (8a, 8b), stating that, for a given x, due to the impurity-size effect, ε decreases (↘) with an increasing (↗) $r_{d(a)}$, and then by **(ii)** the generalized Mott critical d(a)-density defined in the metal-insulator transition (MIT), $N_{CDn(NDp)}(r_{d(a)}, x)$, as observed in Equations (8c, 9a). Furthermore, we also showed that $N_{CDn(NDp)}$ is just the density of carriers localized in exponential band tails, with a precision of the order of 2.89×10^{-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: $Si_{1-x}Ge_x$- 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 $\mathbf{X(x)} \equiv \mathbf{Si_{1-x}Ge_x}$- 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: $r_{do(ao)}$=$r_{Si(Si)}$=0.117 nm (0.117 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:

$$m_{c(v)}(x)/m_o = 0.12\ (0.3) \times x + 0.37353(0.54038) \times (1 - x) \tag{1}$$

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

$$\varepsilon_o(x) = 15.8 \times x + 11.4 \times (1 - x). \tag{2}$$

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

$$E_{go}(x) = 0.7412 \times x + 1.17 \times (1 - x). \tag{3}$$

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

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

and then, the isothermal bulk modulus, by:

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

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

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

At $r_{d(a)} = r_{do(ao)}$, the needed boundary conditions are found to be, for the impurity-atom volume $V= (4\pi/3)\times\left(r_{d(a)}\right)^3$, $V_{do(ao)} = (4\pi/3)\times\left(r_{do(ao)}\right)^3$, for the pressure p, $p_o = 0$, and for the deformation potential energy (or the strain energy) σ, $\sigma_o = 0$. Further, the two important equations[1,7], used to determine the σ-variation, $\Delta\sigma \equiv \sigma - \sigma_o = \sigma$, are defined by: $\frac{dp}{dV} = -\frac{B}{V}$ and $p = -\frac{d\sigma}{dV}$. giving: $\frac{d}{dV}\left(\frac{d\sigma}{dV}\right) = \frac{B}{V}$. Then, by an integration, one gets:

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

Furthermore, we also shown that, as $r_{d(a)} > r_{do(ao)}$ ($r_{d(a)} < r_{do(ao)}$), the compression (dilatation) gives rise to the increase (the decrease) in the energy gap $E_{gn(gp)}\left(r_{d(a)}, x\right)$, and the effective donor (acceptor)-ionization energy $E_{d(a)}\left(r_{d(a)}, x\right)$ 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 $r_{d(a)} \leq r_{do(ao)}$,

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

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

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

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

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

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

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

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

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

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

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

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

This excellent one can be explained from the definition of the reduced effective Wigner-Seitz (**WS**) radius $r_{sn1(sp1)}$, characteristic of interactions, by:

$$r_{sn1(sp1)}(N, r_{d(a)}, x) \equiv \left(\frac{3}{4\pi N}\right)^{1/3} \times \frac{1}{a_{Bn(Bp)}(r_{d(a)}, x)} = 1.1723 \times 10^8 \times \left(\frac{1}{N}\right)^{1/3} \times \frac{m_{c(v)}(x)/m_o}{\varepsilon(r_{d(a)}, x)}, \quad (9b)$$

being equal to, in particular, at N= $N_{CDn(CDp)}(r_{d(a)}, x)$: $r_{sn1(sp1)}\left(N_{CDn(CDp)}(r_{d(a)}, x), r_{d(a)}, x\right) =$ **2.4814015**, for any ($r_{d(a)}, x$)-values. So, from Equations (9a, 9b), one obtains:

$$N_{CDn(CDp)}(r_{d(a)}, x)^{1/3} \times a_{Bn(Bp)}(r_{d(a)}, x) = \left(\frac{3}{4\pi}\right)^{\frac{1}{3}} \times \frac{1}{2.4814015} = \mathbf{0.25} = \mathbf{(WS)_{n(p)}} = \mathbf{M_{n(p)}}. \quad (9c)$$

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

Furthermore, by using $M_{n(p)} = 0.25$, according to the empirical Heisenberg parameter, $\boldsymbol{\mathcal{H}_{n(p)}} = \mathbf{0.47137}$, as given in Equtions (8a, 8b, 8c, 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 $\mathbf{2.89 \times 10^{-7}}$. 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:

$$E_{gni(gpi)}(r_{d(a)}, x, T) \text{ in eV} = E_{gno(gpo)}(r_{d(a)}, x) - 10^{-4} \times T^2 \times \left\{\frac{3.525 \times x}{T+94\ K} + \frac{2.54 \times (1-x)}{T+204\ K}\right\}, \quad (10)$$

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:

$$N_{c(v)}(T, x) = 2 \times g_{c(v)}(x) \times \left(\frac{m_r(x) \times k_B T}{2\pi\hbar^2}\right)^{\frac{3}{2}} (cm^{-3}),\ g_{c(v)}(x) \equiv 4(2) \times x + 6(2) \times (1-x), \quad (11)$$

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 $m_r(x)$, and $\frac{1}{N}$ by $\frac{g_{c(v)}(x)}{N^*}$, the effective Wigner-Seitz radius now 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:

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

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

$$\Delta E_{gn}(N^*, r_d, x) = \Delta E_{gno}(N^*, r_d, x) \times \{0.6 \times x + 1.3 \times (1 - x)\}, \quad (14n)$$

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:

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

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

$$\Delta E_{gp}(N^*, r_a, x) = \Delta E_{gpo}(N^*, r_a, x) \times \{5.2 \times x + 6 \times (1 - x)\}, \quad (14p)$$

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

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

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: $E_{gn1(gp1)}(r_{d(a)}, x) = E_{gno(gpo)}(r_{d(a)}, x)$, according to: $N = N_{CDn(NDp)}(r_{d(a)}, x)$.

OPTICAL COEFFICIENTS

The optical properties of any medium can be described by the complex refraction index $\mathbb{N}$ and the complex dielectric function ε, $\mathbb{N} \equiv n - i\kappa$ and $\varepsilon \equiv \varepsilon_1 - i\varepsilon_2$, where $i^2 = -1$ and $\varepsilon \equiv \mathbb{N}^2$. Therefore, the real and imaginary parts of ε denoted by ε_1 and ε_2 can thus be expressed in terms of the refraction index n and the extinction coefficient κ as: $\varepsilon_1 \equiv n^2 - \kappa^2$ and $\varepsilon_2 \equiv 2n\kappa$. One notes that the optical absorption coefficient α is related to ε_2, n, κ, and the optical conductivity σ_O, by[2]

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

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

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

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

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

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

Then, one has:

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

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

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

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

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

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

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

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

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

Here, the other parameters are determined by: $X_i(E_{gn1(gp1)}) = \frac{A_i}{Q_i} \times \left[-\frac{B_i^2}{2} + E_{gn1(gp1)} B_i - E_{gn1(gp1)}^2 + C_i\right]$,

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

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

NUMERICAL RESULTS

Now, some numerical results of those optical functions are investigated in the n(p)-type $\mathbf{X(x) \equiv Si_{1-x}Ge_x}$- crystalline alloy, as follows.

A. Metal-insulator transition (MIT)-case

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

Then, in this MIT-case, if $E = E_{gn1(gp1)}(r_{d(a)}, x) = E_{gno(gpo)}(r_{d(a)}, x)$, which can be defined as the critical photon energy: $E \equiv E_{CPE}(r_{d(a)}, x)$, one obtains: $\kappa_{MIT}(r_{d(a)}, x) = 0$ from Eq. (20), and from Eq. (16): $\varepsilon_{2(MIT)}(r_{d(a)}, x) = 0$, $\sigma_{O(MIT)}(r_{d(a)}, x) = 0$ and $\alpha_{MIT}(r_{d(a)}, x) = 0$, and the other functions such as : $n_{MIT}(r_{d(a)}, x)$ from Eq. (21), and $\varepsilon_{1(MIT)}(r_{d(a)}, x)$ and $R_{MIT}(r_{d(a)}, x)$ from Eq. (16) decrease with increasing $r_{d(a)}$ and E_{CPE}, as those investigated in Table 1 in Appendix 1.

B. Optical coefficients, obtained as E → ∞

In Eq. (21), at any T, the choice of the real refraction index: $n(E \to \infty, r_{d(a)}, x, T) = n_\infty(r_{d(a)}, x) = \sqrt{\varepsilon(r_{d(a)}, x)} \times \frac{\omega_T}{\omega_L}$, $\omega_T = 5.1 \times 10^{13}\ s^{-1}$ [5] and $\omega_L = 8.9755 \times 10^{13}\ s^{-1}$, was obtained from the Lyddane-Sachs-Teller relation[5], from which T(L) represent the transverse (longitudinal) optical phonon modes. Then, from Equations (16, 17, 20), from such the asymptotic behavior ($E \to \infty$), we obtain: $\kappa_\infty(r_{d(a)}, x) \to 0$ and $\varepsilon_{2,\infty}(r_{d(a)}, x) \to 0$, as E^{-1}, so that $\varepsilon_{1,\infty}(r_{d(a)}, x)$, $\sigma_{O,\infty}(r_{d(a)}, x)$, $\alpha_\infty(r_{d(a)}, x)$ and $R_\infty(r_{d(a)}, x)$ go to their appropriate limiting constants, 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 $\mathbf{X(x)} \equiv \mathbf{Si_{1-x}Ge_x}$- 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 $\mathbf{2.89 \times 10^{-7}}$, 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	Si	Sb	Sn
r_d (nm) [4]	↗	0.110	0.118	0.136	0.140
At **x=0**,					
E_{CPE} in meV	↗	1168.8	1170	1180	1185
n_{MIT}	↘	3.510	3.494	3.381	3.335
$\varepsilon_{1(MIT)}$	↘	12.32	12.21	11.43	11.12
R_{MIT}	↘	0.310	0.308	0.295	0.290
At **x=0.5**,					
E_{CPE} in meV	↗	955.03	955.6	960.3	962.6
n_{MIT}	↘	3.821	3.804	3.685	3.636
$\varepsilon_{1(MIT)}$	↘	14.60	14.47	13.58	13.22
R_{MIT}	↘	0.342	0.341	0.328	0.323
At **x=1**,					
E_{CPE} in meV	↗	741	741.2	742.9	743.7
n_{MIT}	↘	4.119	4.101	3.974	3.923
$\varepsilon_{1(MIT)}$	↘	16.97	16.82	15.79	15.39
R_{MIT}	↘	0.371	0.369	0.357	0.352

Acceptor		B	Si	In	Cd
r_a (nm)	↗	0.088	0.126	0.144	0.148
At **x=0**,					
E_{CPE} in meV	↗	1142.2	1170	1200	1210.8
n_{MIT}	↘	3.864	3.494	3.279	3.224
$\varepsilon_{1(MIT)}$	↘	14.93	12.21	10.75	10.4
R_{MIT}	↘	0.347	0.308	0.284	0.277
At **x=0.5**,					
E_{CPE} in meV	↗	940.4	955.6	972.2	977.9
n_{MIT}	↘	4.199	3.804	3.580	3.524
$\varepsilon_{1(MIT)}$	↘	17.63	14.47	12.82	12.42
R_{MIT}	↘	0.379	0.341	0.317	0.311
At **x=1**,					

E_{CPE} in meV	↗	733.2	741.2	750	753
n_{MIT}	↘	4.521	4.101	3.865	3.807
$\varepsilon_{1(MIT)}$	↘	20.44	16.82	14.94	14.49
R_{MIT}	↘	0.407	0.369	0.347	0.341

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	Si	Sb	Sn
At **x=0**,					
n_{∞}	↘	1.934	1.918	1.812	1.769
$\varepsilon_{1,\infty}$	↘	3.740	3.681	3.282	3.129
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	8.824	8.754	8.267	8.071
$\propto_{\infty}$ in $(10^9 \times cm^{-1}) = 2.1602$					
R_{∞}	↘	0.101	0.099	0.083	0.077
At **x=0.5**,					
n_{∞}	↘	2.112	2.095	1.979	1.932
$\varepsilon_{1,\infty}$	↘	4.461	4.391	3.915	3.732
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	9.638	9.561	9.029	8.815
$\propto_{\infty}$ in $(10^9 \times cm^{-1}) = 2.1602$					
R_{∞}	↘	0.128	0.125	0.108	0.101
At **x=1**,					
n_{∞}	↘	2.277	2.259	2.133	2.082
$\varepsilon_{1,\infty}$	↘	5.183	5.101	4.549	4.336
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	10.388	10.306	9.732	9.502
$\propto_{\infty}$ in $(10^9 \times cm^{-1}) = 2.1602$					
R_{∞}	↘	0.152	0.149	0.131	0.123

Acceptor		B	Si	In	Cd
At **x=0**,					
n_{∞}	↘	2.271	1.918	1.723	1.675
$\varepsilon_{1,\infty}$	↘	5.159	3.681	2.967	2.805
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	10.36	8.75	7.86	7.64
$\propto_{\infty}$ in $(10^9 \times cm^{-1}) = 2.1602$					
R_{∞}	↘	0.151	0.099	0.070	0.064
At **x=0.5**,					
n_{∞}	↘	2.481	2.095	1.881	1.829

$\varepsilon_{1,\infty}$	↘	6.154	4.391	3.540	3.346
$\sigma_{O,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	11.32	9.56	8.58	8.35
$\propto_{\infty}$ in $(10^9\times cm^{-1})=2.1602$					
R_{∞}	↘	0.181	0.125	0.093	0.086

At **x=1**,

n_{∞}	↘	2.674	2.259	2.028	1.972
$\varepsilon_{1,\infty}$	↘	7.150	5.101	4.113	3.887
$\sigma_{O,\infty}$ in $\frac{10^5}{\Omega\times cm}$	↘	12.20	10.31	9.25	8.997
$\propto_{\infty}$ in $(10^9\times cm^{-1})=2.1602$					
R_{∞}	↘	0.207	0.149	0.115	0.107

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,				
$\mathbf{E_{CPE}=1.1688}$	**3.5098**	**0**	**12.3191**	**0**
2	4.288	0.197	18.351	1.690
2.5	5.168	0.671	26.264	6.935
3	4.897	2.754	16.396	26.980
3.5	3.584	2.830	4.835	20.283
4	3.761	2.426	8.260	18.252
4.5	4.197	3.611	4.574	30.310
5	2.039	4.906	−19.917	20.008
5.5	0.626	3.393	−11.120	4.251
6	0.825	2.488	−5.511	4.104
…				
$\mathbf{10^{22}}$	**1.9338**	**0**	**3.7396**	**0**
At x=0.5,				
$\mathbf{E_{CPE}=0.9550}$	**3.8214**	**0**	**14.6032**	**0**
2	4.884	0.163	23.830	1.594
2.5	5.901	0.904	34.005	10.665
3	5.403	3.435	17.392	37.119
3.5	3.764	3.372	2.794	25.389
4	3.969	2.806	7.877	22.278
4.5	4.458	4.089	3.148	36.458
5	2.041	5.469	−25.747	22.328
5.5	0.507	3.736	−13.702	3.786

6	0.754	2.713	−6.792	4.093
…				
10^{22}	**2.1122**	**0**	**4.4613**	**0**
At x=1,				
$E_{CPE} = 0.7410$	**4.1192**	**0**	**16.9680**	**0**
2	5.501	0.122	30.251	1.347
2.5	6.663	1.171	43.024	15.610
3	5.902	4.192	17.260	49.479
3.5	3.907	3.964	−0.444	30.974
4	4.145	3.215	6.850	26.655
4.5	4.693	4.598	0.884	43.160
5	2.005	6.063	−32.745	24.316
5.5	0.345	4.096	−16.661	2.829
6	0.647	2.948	−8.273	3.817
…				
10^{22}	**2.2766**	**0**	**5.1830**	**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} =1.1422	**3.8638**	**0**	**14.9294**	**0**
2	4.676	0.193	21.825	1.809
2.5	5.572	0.698	30.566	7.778
3	5.275	2.835	19.789	29.909
3.5	3.923	2.895	7.009	22.710
4	4.103	2.472	10.727	20.287
4.5	4.545	3.669	7.198	33.351
5	2.356	4.975	−19.199	23.439
5.5	0.928	3.435	−10.935	6.378
6	1.132	2.515	−5.046	5.697
…				
10^{22}	**2.2713**	**0**	**5.1586**	**0**
At x=0.5,				
E_{CPE} =0.9404	**4.1991**	**0**	**17.6324**	**0**
2	5.283	0.160	27.881	1.697

2.5	6.309	0.921	38.955	11.619
3	5.794	3.484	21.431	40.377
3.5	4.132	3.411	5.435	28.191
4	4.339	2.833	10.798	24.589
4.5	4.831	4.123	6.343	39.841
5	2.397	5.509	−24.603	26.408
5.5	0.854	3.760	−13.410	6.422
6	1.105	2.729	−6.226	6.031
…				
10^{22}	**2.4808**	**0**	**6.1542**	**0**
At x=1,				
E_{CPE} =0.7294	**3.8215**	**0**	**14.6036**	**0**
2	5.222	0.120	27.254	1.254
2.5	6.392	1.187	39.445	15.172
3	5.615	4.235	13.595	47.560
3.5	3.600	3.997	−3.013	28.783
4	3.841	3.238	4.268	24.871
4.5	4.392	4.626	−2.117	40.637
5	1.689	6.096	−34.316	20.589
5.5	0.022	4.116	−16.944	0.180
6	0.327	2.961	−8.662	1.936
…				
10^{22}	**1.9716**	**0**	**3.8873**	**0**
E in eV	n	κ	ε_1	ε_2

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

N (10^{18} cm^{-3}) ↗	15	26	60	100
		x=0		
For $\mathbf{r_d} = \mathbf{r_{Si}}$,				
$\eta_n \gg 1$ ↗	14.5	22.9	42.6	60.9
E_{gn1} in eV ↗	1.1527	1.1534	1.160	1.170
n ↘	4.398	4.397	4.391	4.382
κ ↘	3.107	3.105	3.084	3.054
ε_1 ↗	9.684	9.692	9.768	9.876
ε_2 ↘	27.330	27.307	27.085	26.770

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

$\eta_n \gg 1$	↗	13.2	21.9	41.8	60.3
E_{gn1} in eV	↗	1.165	1.166	1.175	1.187
n	↘	4.280	4.279	4.271	4.261
κ	↘	3.071	3.066	3.039	3.004
ε_1	↗	8.891	8.908	9.005	9.128
ε_2	↘	26.287	26.240	25.963	25.604

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

$\eta_n \gg 1$	↗	12.5	21.3	41.4	59.9
E_{gn1} in eV	↗	1.170	1.172	1.182	1.194
n	↘	4.232	4.231	4.222	4.211
κ	↘	3.054	3.048	3.019	2.983
ε_1	↗	8.588	8.607	8.712	8.841
ε_2	↘	25.850	25.795	25.499	25.124

x=0.5

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

$\eta_n \gg 1$	↗	27.5	40.1	70.8	99.8
E_{gn1} in eV	↗	0.929	0.930	0.941	0.955
n	↘	4.765	4.764	4.755	4.743
κ	↘	3.821	3.817	3.783	3.735
ε_1	↗	8.099	8.123	8.299	8.548
ε_2	↘	36.416	36.364	35.980	35.430

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

$\eta_n \gg 1$	↗	27.1	39.9	70.6	99.6
E_{gn1} in eV	↗	0.940	0.942	0.956	0.973
n	↘	4.640	4.638	4.626	4.611
κ	↘	3.790	3.780	3.734	3.676
ε_1	↗	7.168	7.221	7.459	7.755
ε_2	↘	35.172	35.059	34.549	33.900

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

$\eta_n \gg 1$	↗	26.97	39.7	70.5	99.5
E_{gn1} in eV	↗	0.943	0.947	0.962	0.980
n	↘	4.590	4.587	4.574	4.558
κ	↘	3.776	3.764	3.714	3.652

ε_1	↗ 6.807	6.871	7.132	7.446
ε_2	↘ 34.668	34.533	33.977	33.292
		x=1		
For $\mathbf{r_d} = \mathbf{r_{Si}}$,				
$\eta_n \gg 1$	↗ 59.4	85.8	150	210.9
E_{gn1} in eV	↗ 0.690	0.692	0.710	0.737
n	↘ 5.121	5.120	5.106	5.084
κ	↘ 4.668	4.662	4.596	4.497
ε_1	↗ 4.434	4.481	4.947	5.630
ε_2	↘ 47.819	47.738	46.935	45.731
For $\mathbf{r_d} = \mathbf{r_{Sb}}$,				
$\eta_n \gg 1$	↗ 59.35	85.79	149.97	210.88
E_{gn1} in eV	↗ 0.704	0.710	0.737	0.771
n	↘ 4.985	4.980	4.959	4.931
κ	↘ 4.617	4.596	4.498	4.373
ε_1	↗ 3.529	3.681	4.356	5.193
ε_2	↘ 46.032	45.776	44.617	43.137
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,				
$\eta_n \gg 1$	↗ 59.35	85.77	149.95	210.87
E_{gn1} in eV	↗ 0.710	0.717	0.747	0.784
n	↘ 4.930	4.924	4.900	4.870
κ	↘ 4.597	4.570	4.461	4.326
ε_1	↗ 3.171	3.362	4.115	5.007
ε_2	↘ 45.328	45.007	43.720	42.140
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^{19} cm^{-3}) ↗	4	6	8	10
		x=0		
For $\mathbf{r_a} = \mathbf{r_{Si}}$,				

$\eta_p \gg 1$	↗	56.7	80.6	101.3	120.1
E_{gp1} in eV	↗	1.137	1.146	1.156	1.167
n	↘	4.411	4.403	4.395	4.385
κ	↘	3.155	3.128	3.097	3.065
ε_1	↗	9.506	9.608	9.722	9.839
ε_2	↘.	27.834	27.547	27.219	26.879
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↗	42.4	68.97	91.1	110.7
E_{gp1} in eV	↗	1.174	1.186	1.200	1.213
n	↘	4.183	4.172	4.160	4.148
κ	↘	3.042	3.006	2.966	2.926
ε_1	↗	8.240	8.371	8.512	8.650
ε_2	↘.	25.455	25.086	24.681	24.274
For $\mathbf{r_a} = \mathbf{r_{Cd}}$,					
$\eta_p \gg 1$	↗	36.2	64.21	86.96	107
E_{gp1} in eV	↗	1.184	1.197	1.211	1.226
n	↘	4.126	4.115	4.102	4.090
κ	↘	3.012	2.974	2.932	2.889
ε_1	↗	7.955	8.088	8.234	8.376
ε_2	↘.	24.852	24.476	24.055	23.634
			x=0.5		
For $\mathbf{r_a} = \mathbf{r_{Si}}$,					
$\eta_p \gg 1$	↗	94.99	126.8	155	180.8
E_{gp1} in eV	↗	0.886	0.892	0.901	0.911
n	↘	4.800	4.795	4.788	4.800
κ	↘	3.968	3.946	3.916	3.883
ε_1	↗	7.296	7.419	7.585	7.771
ε_2	↘.	38.103	37.849	37.505	37.116
For $\mathbf{r_a} = \mathbf{r_{In}}$,					
$\eta_p \gg 1$	↗	90.10	122.6	151	177
E_{gp1} in eV	↗	0.928	0.941	0.956	0.971
n	↘	4.552	4.541	4.529	4.516
κ	↘	3.826	3.782	3.733	3.683
ε_1	↗	6.082	6.318	6.574	6.831

ε_2	↘.	34.831	34.345	33.812	33.265
For $\mathbf{r_a = r_{Cd}}$,					
$\eta_p \gg 1$	↗	88.18	120.9	150	176
E_{gp1} in eV	↗	0.939	0.953	0.969	0.986
n	↘	4.491	4.478	4.465	4.451
κ	↘	3.790	3.741	3.688	3.634
ε_1	↗	5.801	6.061	6.334	6.605
ε_2	↘.	34.041	33.509	32.937	32.358
			x=1		
For $\mathbf{r_a = r_{Si}}$,					
$\eta_p \gg 1$	↗	179.6	236	286.9	333
E_{gp1} in eV	↗	0.629	0.641	0.657	0.675
n	↘	5.169	5.160	5.148	5.134
κ	↘	4.898	4.853	4.794	4.728
ε_1	↗	2.728	3.074	3.519	4.005
ε_2	↘.	50.638	50.081	49.354	48.544
For $\mathbf{r_a = r_{In}}$,					
$\eta_p \gg 1$	↗	177.6	234.6	285	332
E_{gp1} in eV	↗	0.694	0.719	0.746	0.774
n	↘	4.888	4.868	4.846	4.824
κ	↘	4.655	4.561	4.463	4.363
ε_1	↗	2.222	2.890	3.573	4.240
ε_2	↘.	45.509	44.411	43.257	42.096
For $\mathbf{r_a = r_{Cd}}$,					
$\eta_p \gg 1$	↗	176.8	233.9	284.7	331
E_{gp1} in eV	↗	0.709	0.738	0.767	0.797
n	↘	4.820	4.797	4.773	4.749
κ	↘	4.599	4.495	4.387	4.280
ε_1	↗	2.079	2.810	3.538	4.237
ε_2	↘.	44.330	43.123	41.885	40.655
N (10^{19} cm^{-3})	↗	4	6	8	10

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 η_n ($\gg 1$, 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 $r_d = r_{Si}$,					
$\eta_n \gg 1$	↘	61	24	12	4
E_{gn1} in eV	↘	1.1702	1.168	1.162	1.120
n	↗	4.382	4.384	4.390	4.426
κ	↗	3.054	3.061	3.080	3.208
ε_1	↘	9.876	9.852	9.784	9.299
ε_2	↗	26.770	26.839	27.040	28.402
For $r_d = r_{Sb}$,					
$\eta_n \gg 1$	↘	60.3	24	12	3.80
E_{gn1} in eV	↘	1.187	1.185	1.178	1.136
n	↗	4.261	4.263	4.268	4.305
κ	↗	3.004	3.011	3.030	3.157
ε_1	↘	9.128	9.106	9.039	8.565
ε_2	↗	25.604	25.670	25.865	27.186
For $r_d = r_{Sn}$,					
$\eta_n \gg 1$	↘	60	23.9	11.92	3.77
E_{gn1} in eV	↘	1.194	1.192	1.186	1.143
n	↗	4.211	4.213	4.219	4.256
κ	↗	2.983	2.989	3.008	3.135
ε_1	↘	8.841	8.819	8.753	8.284
ε_2	↗	25.124	25.189	25.381	26.686
x=0.5					
For $r_d = r_{Si}$,					
$\eta_n \gg 1$	↘	99.8	39.9	19.9	6.53
E_{gn1} in eV	↘	0.955	0.952	0.943	0.890
n	↗	4.743	4.746	4.754	4.797
κ	↗	3.735	3.747	3.777	3.956
ε_1	↘	8.548	8.488	8.329	7.368

ε_2	↗	35.430	35.564	35.915	37.954
For $\mathbf{r_d} = \mathbf{r_{Sb}}$,					
$\eta_n \gg 1$	↘	99.6	39.8	19.89	6.51
E_{gn1} in eV	↘	0.973	0.970	0.960	0.908
n	↗	4.611	4.614	4.622	4.666
κ	↗	3.676	3.687	3.718	3.895
ε_1	↘	7.755	7.697	7.542	6.603
ε_2	↗	33.900	34.030	34.369	36.345
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↘	99.5	39.8	19.87	6.509
E_{gn1} in eV	↘	0.980	0.977	0.968	0.915
n	↗	4.558	4.561	4.569	4.613
κ	↗	3.652	3.663	3.694	3.870
ε_1	↘	7.446	7.388	7.234	6.304
ε_2	↗	33.292	33.420	33.755	35.705
x=1					
For $\mathbf{r_d} = \mathbf{r_{Si}}$,					
$\eta_n \gg 1$	↘	210.9	84.3	42.2	14
E_{gn1} in eV	↘	0.737	0.732	0.720	0.656
n	↗	5.084	5.088	5.098	5.148
κ	↗	4.497	4.515	4.560	4.797
ε_1	↘	5.630	5.508	5.201	3.495
ε_2	↗	45.731	45.949	46.492	49.392
For $\mathbf{r_d} = \mathbf{r_{Sb}}$,					
$\eta_n \gg 1$	↘	210.88	84.3	42.16	14
E_{gn1} in eV	↘	0.771	0.766	0.754	0.690
n	↗	4.931	4.935	4.945	4.996
κ	↗	4.373	4.391	4.435	4.669
ε_1	↘	5.193	5.076	4.784	3.156
ε_2	↗	43.137	43.346	43.867	46.654
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,					
$\eta_n \gg 1$	↘	210.87	84.3	42.15	14
E_{gn1} in eV	↘	0.784	0.779	0.767	0.703

n	↗	4.870	4.874	4.884	4.935
κ	↗	4.326	4.344	4.387	4.620
ε_1	↘	5.007	4.892	4.605	3.006
ε_2	↗	42.140	42.346	42.859	45.602
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 $\eta_p (\gg 1, degenerate\ case)$, 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 $\mathbf{r_a = r_{Si}}$,					
$\eta_p \gg 1$	↘	120.1	48.02	23.98	7.90
E_{gp1} in eV	↘	1.167	1.165	1.158	1.119
n	↗	4.385	4.387	4.392	4.427
κ	↗	3.065	3.071	3.089	3.210
ε_1	↘	9.839	9.816	9.750	9.293
ε_2	↗	26.879	26.946	27.140	28.419
For $\mathbf{r_a = r_{In}}$,					
$\eta_p \gg 1$	↘	110.7	44.29	22.11	7.30
E_{gp1} in eV	↘	1.213	1.211	1.205	1.165
n	↗	4.148	4.150	4.156	4.190
κ	↗	2.926	2.932	2.950	3.068
ε_1	↘	8.650	8.629	8.568	8.146
ε_2	↗	24.274	24.336	24.517	25.715
For $\mathbf{r_a = r_{Cd}}$,					
$\eta_p \gg 1$	↘	107	42.80	21.37	7.02
E_{gp1} in eV	↘	1.226	1.224	1.217	1.178
n	↗	4.090	4.091	4.097	4.132
κ	↗	2.889	2.896	2.914	3.031
ε_1	↘	8.376	8.356	8.296	7.882
ε_2	↗	23.634	23.696	23.834	25.053
			x=0.5		

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

$\eta_p \gg 1$	↘	180.8	72.31	36.14	11.98
E_{gp1} in eV	↘	0.911	0.908	0.899	0.847
n	↗	4.780	4.783	4.790	4.832
κ	↗	3.883	3.894	3.925	4.102
ε_1	↘	7.771	7.706	7.536	6.521
ε_2	↗	37.116	37.253	37.608	39.648

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

$\eta_p \gg 1$	↘	177.3	70.91	35.44	11.75
E_{gp1} in eV	↘	0.971	0.967	0.958	0.907
n	↗	4.516	4.519	4.527	4.569
κ	↗	3.683	3.694	3.725	3.897
ε_1	↘	6.831	6.772	6.617	5.691
ε_2	↗	33.265	33.391	33.721	35.615

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

$\eta_p \gg 1$	↘	175.9	70.36	35.16	11.66
E_{gp1} in eV	↘	0.986	0.982	0.973	0.922
n	↗	4.451	4.454	4.462	4.505
κ	↗	3.634	3.646	3.676	3.847
ε_1	↘	6.605	6.547	6.396	5.491
ε_2	↗	32.358	32.482	32.806	34.665

x=1

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

$\eta_p \gg 1$	↘	333	133	66.65	22.18
E_{gp1} in eV	↘	0.675	0.670	0.658	0.594
n	↗	5.134	5.138	5.147	5.196
κ	↗	4.728	4.746	4.792	5.033
ε_1	↘	4.005	3.871	3.533	1.671
ε_2	↗	48.544	48.770	49.329	52.306

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

$\eta_p \gg 1$	↘	332	132.7	66.35	22.08
E_{gp1} in eV	↘	0.774	0.769	0.757	0.694
n	↗	4.824	4.828	4.838	4.888

κ	↗	4.363	4.380	4.424	4.656
ε_1	↘	4.240	4.124	3.832	2.214
ε_2	↗	42.096	42.301	42.810	45.522

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

$\eta_p \gg 1$	↘	331	132.5	66.24	22.05
E_{gp1} in eV	↘	0.797	0.792	0.780	0.716
n	↗	4.749	4.753	4.763	4.813
κ	↗	4.280	4.297	4.341	4.571
ε_1	↘	4.237	4.125	3.843	2.279
ε_2	↗	40.655	40.856	41.353	44.003
T in K	↗	20	50	100	300