wjert, 2024, Vol. 10 Issue 5, 80-106. Review Article ISSN 2454-695X

World Journal of Engineering Research and Technology
WJERT
www.wjert.org
SJIF Impact Factor: 7.029

NEW CRITICAL DENSITY IN METAL-INSULATOR TRANSITION, OBTAINED IN n(p)-TYPE DEGENERATE, Si(1-x)Ge(x)-CRYSTALLINE ALLOY, AND ITS APPLICATIONS. (V)

Prof. Dr. Huynh Van Cong*

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

Article Received on 04/03/2024 **Article Revised on 24/03/2024** **Article Accepted on 14/04/2024**

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

ABTRACT

In n(p)-type degenerate X(x) $\equiv [Si_{1-x}(Ge_x)] -$ crystalline alloy, $0 \leq x \leq 1$, by basing on the same physical model and treatment method, as used in our recent works.[1,2] we will investigate **(1)**-the critical impurity densities in the Mott metal-insulator transition (Mott-MIT), $N_{CDn(CDp)}$, determined in Eq. (8), and **the origin of this Mott's criterium, Eq. (8)**, being investigated in Eq. (9b), **(2)**-the density of electrons (holes) localized in the exponential conduction (valence)-band tails (EBT), $N^{EBT}_{CDn(CDp)}(r_{d(a)},x)$, given in Eq. (26), giving rise to: $N^{EBT}_{CDn(CDp)}(r_{d(a)},x) \cong N_{CDn(CDp)}(r_{d(a)},x)$, with a precision of the order of 2.89×10^{-7}, as observed in Tables 1n and 1p, which could be concluded that $N_{CDn(CDp)}$ **is also the density of electrons (holes) localized in the EBT**, and **(3)**-the optical band gap, $E_{gn1(gp1)}(N^*,r_{d(a)},x,T)$, determined in Eq. (28), $N^*(N,r_{d(a)},x) \equiv N - N_{CDn(NDp)}$, showing that the numerical results of $E_{gn1(gp1)}(N^*,r_{d(a)},x=0,T=20\,K)$ are in good agreement with experimental ones, obtained by Wagner and del Alamo (1988), with maximal relative deviations: 5.38 % (9.07 %), and 2.06 % (5.16 %), as observed in Tables 2n and 2p; further, for x(=0, 0.5, 1), the numerical results of $E_{gn1(gp1)}(N^*,r_{d(a)},x,T=20\,K)$ are given in Tables 3n and 3p.

KEYWORS: $Si_{1-x}Ge_x$- crystalline alloy; critical impurity density in the Mott MIT; optical band gap.

INTRODUCTION

By basing on the same intrinsic energy-band-structure parameters, physical model and treatment method, as used in our recent work,[1] and also other works,[2-12] we will investigate the critical impurity density in the metal-insulator transition (MIT), obtained in the n(p)-type degenerate X(x)≡ $[Si_{1-x}(Ge_x)]$crystalline alloy, $0 \le x \le 1$, being due to the effects of the size of donor (acceptor) d(a)-radius, $r_{d(a)}$, the x- concentration, and finally the high d(a)-density, N, assuming that all the impurities are ionized even at T=0 K. In such n(p)-type degenerate crystalline alloy, we will determine.

(i)- the critical total impurity density $N_{CDn(CDp)}(r_{d(a)},x)$ in the Mott-MIT, in which the assumption of the one conduction (valence)-band was used, as that given in Eq.[8] using an empirical Mott parameter $M_{n(p)} = 0.25$, and the density of electrons (holes) localized in the exponential conduction(valence)-band tails (EBT), $N^{EBT}_{CDn(CDp)}(r_{d(a)},x)$, as that given in Eq.[26] with the use of the empirical Heisenberg parameter $\mathcal{H}_{n(p)}(x) = 0.47137$, as that given in Eq.[15] according to: for given $r_{d(a)}$ and x, $N^{EBT}_{CDn(CDp)}(r_{d(a)},x) \cong N_{CDn(CDp)}(r_{d(a)},x)$, with a precision of the order of 2.89×10^{-7} (2.88×10^{-7}), as seen in Tables 1n and 1p, respectively, being more accurate compared with the corresponding ones 9.99×10^{-6} (1.49×10^{-5}), given in our recent work.[2] in which the assumption of 3-conduction bands and 2-valence bands was taken, and ***(ii)****-the optical band gap* (***OBG***), $E_{gn1(gp1)}(N^*,r_{d(a)},x,T)$, $N^* \equiv N - N_{CDn(NDp)}$, *as that given in Eq.*[28] *in which the effective average number of equivalent conduction (valence)-band edges was used as:* $g_c(x) = 4 \times x + 6 \times (1-x)$, $g_v(x) = 2 \times x + 2 \times (1-x)$*; then, its numerical results are reported in Tables 2n, 2p, 3n and 3p, showing, in particular, in Tables 2n and 2p, in which for* $r_{d(a)} \equiv r_{p(B)}$, *x=0 and T=20 K, the numerical results of* $E_{gn1(gp1)}$ *are found to be in good agreement with the data, obtained by Wagner & del Alamo (1988), with maximal relative deviations: 5.38 % (9.07 %), and 2.06 % (5.16 %), respectively.*

In the following, we will determine those functions: $N_{CDn(CDp)}(r_{d(a)},x)$, $N^{EBT}_{CDn(CDp)}(r_{d(a)},x)$, and finally, $E_{gn1(gp1)}(N^*,r_{d(a)},x,T)$.

CRITICAL DENSITY IN THE MOTT MIT

Such the critical impurity density $N_{CDn(CDp)}(r_{d(a)},x)$, expressed as a function of $r_{d(a)}$ and x, is determined as follows.

Effect of x-concentration

Here, the values of the intrinsic energy-band-structure parameters, such as: the unperturbed relative effective electron (hole) mass in conduction (valence) bands $m_{c(v)}(x)/m_o$, m_o being the electron rest mass, the reduced effective mass $m_r(x)/m_c$, the unperturbed relative dielectric static constant $\varepsilon_o(x)$, the intrinsic energy gap, $E_{go}(x)$

$m_c(x)/m_o = 0.12 \times x + 0.37353 \times (1-x)$, $m_v(x)/m_o = 0.3 \times x + 0.54038 \times (1-x)$,

$m_r(x)/m_o = \frac{m_c(x) \times m_v(x)}{m_c(x)+m_v(x)}$,

$\varepsilon_o(x) = 15.8 \times x + 11.4 \times (1-x)$,

$E_{go}(x)\ \text{in eV} = 0.7412 \times x + 1.17 \times (1-x)$, and the isothermal bulk modulus $B_{do(ao)}(x) \equiv \frac{E_{do(ao)}(x)}{(4\pi/3)\times(r_{do(ao)})^3}$, determined at $r_{d(a)} = r_{do(ao)} = r_{Si(Si)} = 0.117$ nm (0.117 nm).

Therefore, the effective donor (acceptor)-ionization energy $E_{do(ao)}(x)$ and the isothermal bulk modulus $B_{do(ao)}(x)$ are found to be given by:

$$E_{do(ao)}(x) = \frac{13600\times[m_{c(v)}(x)/m_o]}{[\varepsilon_o(x)]^2}\ \text{meV} \quad \text{and} \qquad (1)$$

$$B_{do(ao)}(x) \equiv \frac{E_{do(ao)}(x)}{(4\pi/3)\times(r_{do(ao)})^3}. \qquad (2)$$

Effects of impurity size, with a given x

Here, one shows that the effects of the size of donor (acceptor) d(a)-radius, $r_{d(a)}$, and the x-concentration strongly affects the changes in all the energy-band-structure parameters, which can be represented by the effective relative static dielectric constant $\varepsilon(r_{d(a)},x)$, 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, as: $p_o = 0$, and for the deformation potential energy (or the strain energy) σ, as: $\sigma_o = 0$. Further, the two important equations, 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: $\frac{d}{dV}(\frac{d\sigma}{dV}) = \frac{B}{V}$. Then, by an integration, one gets:

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

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 $E_{gno(gpo)}(r_{d(a)},x)$, and in the effective donor (acceptor)-ionization energy $E_{d(a)}(r_{d(a)},x)$ in the absolute values, being obtained from the effective Bohr model, and then such the compression (dilatation) 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 $r_{d(a)} \leq r_{do(ao)}$,

$$E_{gno(gpo)}(r_{d(a)},x) - E_{go}(x) = E_{d(a)}(r_{d(a)},x) - E_{do(ao)}(x) = E_{do(ao)}(x) \times \left[\left(\frac{\varepsilon_o(x)}{\varepsilon(r_{d(a)})}\right)^2 - 1\right] = -[\Delta\sigma(r_{d(a)},x)]_{n(p)}. \quad (4)$$

Therefore, from above Equations (3) and (4), 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 $\varepsilon(r_{d(a)},x) = \frac{\varepsilon_o(x)}{\sqrt{1+\left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3}} \leq \varepsilon_o(x)$,

$$E_{gno(gpo)}(r_{d(a)},x) - E_{go}(x) = E_{d(a)}(r_{d(a)},x) - E_{do(ao)}(x) = E_{do(ao)}(x) \times \left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 \geq 0, \quad (5)$$

according to the increase in both $E_{gn(gp)}(r_{d(a)},x)$ and $E_{d(a)}(r_{d(a)},x)$, 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: $\left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 < 1$,

$$E_{gno(gpo)}(r_{d(a)},x) - E_{go}(x) = E_{d(a)}(r_{d(a)},x) - E_{do(ao)}(x) = -E_{do(ao)}(x) \times \left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 \leq 0, \quad (6)$$

Corresponding to the decrease in both $E_{gn(gp)}(r_{d(a)},x)$ and $E_{d(a)}(r_{d(a)},x)$, for a given x.

Furthermore, the effective Bohr radius $a_{Bn(Bp)}(r_{d(a)})$ is defined by:

$$a_{Bn(Bp)}(r_{d(a)},x) \equiv \frac{\varepsilon(r_{d(a)},x) \times \hbar^2}{m_{c(v)}(x) \times q^2} = 0.53 \times 10^{-8}\ \text{cm} \times \frac{\varepsilon(r_{d(a)},x)}{m_{c(v)}(x)/m_o}, \quad (7)$$

Where $-q$ is the electron charge.

In the n(p)-type degenerate $Si_{1-x}Ge_x$- crystalline alloy, in which the assumption of one conduction (valence)-band is used, the critical total donor (acceptor)-density in the Mott-MIT, $N_{CDn(NDp)}(r_{d(a)},x)$, is determined by:

$$N_{CDn(CDp)}(r_{d(a)},x)^{1/3} \times a_{Bn(Bp)}(r_{d(a)},x) \simeq M_{n(p)},\ M_{n(p)} = 0.25. \quad (8)$$

Eq. (8) is thus the Mott-criterium, used to determine $N_{CDn(CDp)}$, depending on the choice of empirical parameters, given in Eq. (7), such as: $m_{c(v)}(x)$ or $\varepsilon_o(x)$, so that the numerical results of $N_{CDn(CDp)}(r_{d(a)},x)$, being in good accordance with those, observed in experiments.

In the following, these obtained numerical results can also be justified by calculating those of the density of electrons (holes) localized in exponential conduction (valence)-band (EBT) tails, $N^{EBT}_{CDn(CDp)}(r_{d(a)},x)$.

$N^{EBT}_{CDn(CDp)}(r_{d(a)},x)$- Expression

In order to determine $N^{EBT}_{CDn(CDp)}(r_{d(a)},x)$, we first present our physical model and also our mathematical methods, in such the assumption of one conduction (valence)-band.

Physical model (Origin of the Mott's criterium)

In the n(p)-type degenerate $Si_{1-x}Ge_x$- crystalline alloy, if denoting the Fermi wave number by: $k_{Fn(Fp)}(N) \equiv (3\pi^2 N)^{1/3}$, N being the total impurity density with an assumption that all the impurities are ionized even at temperature T=0 K, the reduced effective Wigner-Seitz (**WS**) radius $r_{sn(sp)}$, characteristic of interactions, is defined by:

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

explaining thus the origin of the excellent Mott's criterium.

Here, one notes that, at $N = N_{CDn(CDp)}(r_{d(a)},x)$, $r_{sn(sp)}(N_{CDn(CDp)}(r_{d(a)},x),r_{d(a)},x) = 2.4852548$, being determined from Eq. (9a), as those also observed in Tables 1n and 1p in Appendix 1. In other words, the above Mott's criterium (8) can also be explained by Eq. (9a), as:

$$N_{CDn(CDp)}(r_{d(a)},x)^{1/3} \times a_{Bn(Bp)}(r_{d(a)},x) = \left(\frac{3}{4\pi}\right)^{1/3} \times \frac{1}{2.4852548} = 0.2496124 = (\mathbf{WS})_{n(p)} \simeq \mathbf{M}_{n(p)} = 0.25$$

, with a relative deviation ($=1.5504 \times 10^{-3}$). (9b)

Then, the ratio of the inverse effective screening length $k_{sn(sp)}$ to Fermi wave number $k_{Fn(kp)}$ is defined by

$$R_{sn(sp)}(N,r_{d(a)},x) \equiv \frac{k_{sn(sp)}}{k_{Fn(Fp)}} = \frac{k^{-1}_{Fn(Fp)}}{k^{-1}_{sn(sp)}} = R_{snWS(spWS)} + \left[R_{snTF(spTF)} - R_{snWS(spWS)}\right]e^{-r_{sn(sp)}} < 1. \quad (10)$$

These ratios, $R_{snTF(spTF)}$ and $R_{snWS(spWS)}$, are determined in the following.

First, for $N \gg N_{CDn(NDp)}(r_{d(a)},x)$, according to the Thomas-Fermi (TF)-approximation, the ratio $R_{snTF(snTF)}$ is reduced to

$$R_{snTF}(N,r_{d(a)},x) \equiv \frac{k_{snTF(spTF)}}{k_{Fn(Fp)}} = \frac{k_{Fn(Fp)}^{-1}}{k_{snTF(spTF)}^{-1}} = \sqrt{\frac{4\gamma r_{sn(sp)}(N,r_{d(a)},x)}{\pi}} \ll 1, \quad (11)$$

being proportional to $N^{-1/6}$.

Secondly, $N < N_{CDn(NDp)}(r_{d(a)})$, according to the Wigner-Seitz (WS)-approximation, the ratio $R_{snWS(spWS)}$ is reduced to [3]:

$$R_{snWS(spWS)}(N,r_{d(a)},x) \equiv \frac{k_{snWS(spWS)}}{k_{Fn(Fp)}} = \left(\frac{s}{2\pi} - \gamma\frac{d\left[r_{sn(sp)}^2 \times E_{CE}\right]}{dr_{sn(sp)}}\right) \times 0.5\,,$$

(12) where $E_{CE}(N,r_{d(a)},x)$ is the majority-carrier correlation energy (CE), being determined by

$$E_{CE}(N,r_{d(a)},x) \equiv \frac{-0.87553}{0.0908+r_{sn(sp)}} + \frac{\frac{0.87553}{0.0908+r_{sn(sp)}} + \left(\frac{2[1-\ln(2)]}{\pi^2}\right)\times\ln(r_{sn(sp)}) - 0.093288}{1+0.0384728\times r_{sn(sp)}^{1.67378876}}\,.$$

So, n(p)-type degenerate $X(x)$- crystalline alloys, the physical conditions are found to be given by :

$$\frac{k_{Fn(Fp)}^{-1}}{a_{Bn(Bp)}} < \frac{\eta_{n(p)}}{E_{Fno(Fpo)}} \equiv \frac{1}{A_{n(p)}} < \frac{k_{Fn(Fp)}^{-1}}{k_{sn(sp)}^{-1}} \equiv R_{sn(sp)}(N,r_{d(a)},x) < 1,\ A_{n(p)}(N,r_{d(a)},x) \equiv \frac{\pm E_{Fn(Fp)}}{\eta_{n(p)}}. \quad (13)$$

Here, $\pm E_{Fn(Fp)}$ is the Fermi energy at 0 K, and $\eta_{n(p)}$ is defined in next Eq. (15), as:

$$\pm E_{Fn(Fp)}(N,x) = \frac{\hbar^2 \times k_{Fn(Fp)}(N)^2}{2\times m_{c(v)}(x)} \geq 0, \eta_{n(p)}(N,r_{d(a)},x) = \frac{\sqrt{2\pi N}}{\varepsilon(r_{d(a)},x)} \times q^2 k_{sn(sp)}^{-1/2}.$$

Then, the total screened Coulomb impurity potential energy due to the attractive interaction between an electron (hole) charge, $-q(+q)$, at position $\vec{r}$, and an ionized donor (ionized acceptor) charge: $+q(-q)$ at position $\overrightarrow{R_j}$, randomly distributed throughout $X(x)$- crystalline alloys, is defined by:

$$V(r) \equiv \sum_{j=1}^{\mathbb{N}} v_j(r) + V_o, \quad (14)$$

where $\mathbb{N}$ is the total number of ionized donors (acceptors), V_o is a constant potential energy, and the screened Coulomb potential energy $v_j(r)$ is defined as:

$$v_j(r) \equiv -\frac{q^2\times\exp(-k_{sn(sp)}\times|\vec{r}-\overrightarrow{R_j}|)}{\varepsilon(r_{d(a)})\times|\vec{r}-\overrightarrow{R_j}|},$$

where $k_{sn(sp)}$ is the inverse screening length determined in Eq. (11).

Further, using a Fourier transform, the v_j-representation in wave vector $\vec{k}$-espace is given by

$$v_j(\vec{k}) = -\frac{q^2}{\varepsilon(r_{d(a)})} \times \frac{4\pi}{\Omega} \times \frac{1}{k^2+k_{sn(sp)}^2},$$

where Ω is the total $X(x)$- crystalline alloy volume.

Then, the effective auto-correlation function for potential fluctuations, $W_{n(p)}(\nu_{n(p)}, N, r_{d(a)}) \equiv \langle V(r)V(r')\rangle$, was determined, [4, 5] as :

$$W_{n(p)}(\nu_{n(p)}, N, r_{d(a)}, x) \equiv \eta^2_{n(p)} \times \exp\left(\frac{-\mathcal{H}_{n(p)} \times R_{sn(sp)}(N, r_{d(a)}, x)}{2\sqrt{|\nu_{n(p)}|}}\right), \eta_{n(p)}(N, r_{d(a)}, x) \equiv \frac{\sqrt{2\pi N}}{\varepsilon(r_{d(a)})} \times q^2 k^{-1/2}_{sn(sp)},$$

$$\nu_{n(p)}(E, N, x) \equiv \frac{\mp E}{\pm E_{Fno(Fpo)}(N,x)}, \ \mathcal{H}_{n(p)} = 0.47137 . \quad (15)$$

Here, E is the total electron energy, and the empirical Heisenberg parameter $\mathcal{H}_{n(p)} = 0.47137$ was chosen above such that the determination of the density of electrons localized in the conduction(valence)-band tails will be accurate, noting that as $E \to \pm\infty$, $|\nu_{n(p)}| \to \infty$, and therefore, $W_{n(p)} \to \eta^2_{n(p)}$.

In the following, we will calculate the ensemble average of the function: $(E - V)^{a-\frac{1}{2}} \equiv E_k^{a-\frac{1}{2}}$, for $a \geq 1$, $E_k \equiv \frac{\hbar^2 \times k^2}{2 \times m_{c(v)}(x)}$ being the kinetic energy of the electron (hole), and $V(r)$ determined in Eq. (16), by using the two following integration methods, which strongly depend on $W_{n(p)}(\nu_{n(p)}, N, r_{d(a)}, x)$.

MATHEMATICAL METHODS

Kane integration method (KIM)

Here, the effective Gaussian distribution probability is defined by:

$$P(V) \equiv \frac{1}{\sqrt{2\pi W_{n(p)}}} \times \exp\left[\frac{-V^2}{2W_{n(p)}}\right]. \quad (16)$$

So, in the Kane integration method, the Gaussian average of $(E - V)^{a-\frac{1}{2}} \equiv E_k^{a-\frac{1}{2}}$ is defined by

$$\langle (E - V)^{a-\frac{1}{2}} \rangle_{KIM} \equiv \langle E_k^{a-\frac{1}{2}} \rangle_{KIM} = \int_{-\infty}^{E} (E - V)^{a-\frac{1}{2}} \times P(V) dV, \quad \text{for } a \geq 1.$$

Then, by variable changes: $s = (E - V)/\sqrt{W_{n(p)}}$ and $y = \mp E/\sqrt{W_{n(p)}} \equiv \frac{\pm E_{Fn(Fp)}}{\eta_{n(p)}} \times \nu_{n(p)} \times \exp\left(\frac{\mathcal{H}_{n(p)} \times R_{sn(sp)}}{4 \times \sqrt{|\nu_{n(p)}|}}\right)$, and using an identity:

$$\int_0^\infty s^{a-\frac{1}{2}} \times \exp(-ys - \tfrac{s^2}{2}) ds \equiv \Gamma(a + \tfrac{1}{2}) \times \exp(y^2/4) \times D_{-a-\frac{1}{2}}(y),$$

where $D_{-a-\frac{1}{2}}(y)$ is the parabolic cylinder function and $\Gamma(a + \frac{1}{2})$ is the Gamma function, one thus has

$$\langle E_k^{a-\frac{1}{2}}\rangle_{KIM} = \frac{\exp(-y^2/4)\times W_{n(p)}^{\frac{2a-1}{4}}}{\sqrt{2\pi}} \times \Gamma(a+\tfrac{1}{2}) \times D_{-a-\frac{1}{2}}(y) = \frac{\exp(-y^2/4)\times \eta_{n(p)}^{a-\frac{1}{2}}}{\sqrt{2\pi}} \times \exp\left(-\frac{\mathcal{H}_{n(p)}\times R_{sn(sp)}\times(2a-1)}{8\times\sqrt{|\nu_{n(p)}|}}\right)\times$$

$$\Gamma(a+\tfrac{1}{2}) \times D_{-a-\frac{1}{2}}(y) \qquad (16)$$

Feynman path-integral method (FPIM)

Here, the ensemble average of $(E-V)^{a-\frac{1}{2}} \equiv E_k^{a-\frac{1}{2}}$ is defined by

$$\langle (E-V)^{a-\frac{1}{2}}\rangle_{FPIM} \equiv \langle E_k^{a-\frac{1}{2}}\rangle_{FPIM} \equiv \frac{\hbar^{a-\frac{1}{2}}}{2^{3/2}\times\sqrt{2\pi}} \times \frac{\Gamma(a+\frac{1}{2})}{\Gamma(\frac{3}{2})} \times \int_{-\infty}^{\infty}(it)^{-a-\frac{1}{2}} \times \exp\left\{\frac{iEt}{\hbar} - \frac{(t\sqrt{W_{n(p)}})^2}{2\hbar^2}\right\} dt,\ i^2=-1,$$

noting that as a=1, $(it)^{-\frac{3}{2}} \times \exp\left\{-\frac{(t\sqrt{W_p})^2}{2\hbar^2}\right\}$ is found to be proportional to the averaged Feynman propagator given the dense donors (acceptors). Then, by variable changes: $t = \frac{\hbar}{\sqrt{W_{n(p)}}}$ and $y = \mp E/\sqrt{W_{n(p)}} \equiv \frac{\pm E_{Fn(Fp)}}{\eta_{n(p)}} \times \nu_{n(p)} \times \exp\left(\frac{\mathcal{H}_{n(p)}\times R_{sn(sp)}}{4\times\sqrt{|\nu_{n(p)}|}}\right)$, for n(p)-type respectively, and then using an identity

$$\int_{-\infty}^{\infty}(is)^{-a-\frac{1}{2}} \times \exp\left\{iys - \frac{s^2}{2}\right\} ds \equiv 2^{3/2} \times \Gamma(3/2) \times \exp(-y^2/4) \times D_{-a-\frac{1}{2}}(y),$$

one finally obtains: $\langle E_k^{a-\frac{1}{2}}\rangle_{FPIM} \equiv \langle E_k^{a-\frac{1}{2}}\rangle_{KIM}$, $\langle E_k^{a-\frac{1}{2}}\rangle_{KIM}$ being determined in Eq. (16).

In the following, with the use of asymptotic forms for $D_{-a-\frac{1}{2}}(y)$, those given for $\langle (E-V)^{a-\frac{1}{2}}\rangle_{KIM}$ can be obtained in the two following cases.

First case: n-type ($E \geq 0$) and p-type ($E \leq 0$)

As $E \to \pm\infty$, one has: $\nu_{n(p)} \to \mp\infty$ and $y \to \mp\infty$. In this case, one gets: $D_{-a-\frac{1}{2}}(y \to \mp\infty) \approx \frac{\sqrt{2\pi}}{\Gamma(a+\frac{1}{2})} \times e^{\frac{y^2}{4}} \times (\mp y)^{a-\frac{1}{2}}$, and therefore from Eq. (16), one gets:

$$\langle E_k^{a-\frac{1}{2}}\rangle_{KIM} \approx E^{a-\frac{1}{2}}. \qquad (17)$$

Further, as $E \to \pm 0$, one has: $\nu_{n(p)} \to \mp 0$ and $y \to \mp 0$. So, one obtains:

$$D_{-a-\frac{1}{2}}(y \to \mp 0) \simeq \beta(a) \times \exp\left((\sqrt{a} + \frac{1}{16a^{\frac{3}{2}}})y - \frac{y^2}{16a} + \frac{y^3}{24\sqrt{a}}\right) \to \beta(a), \quad \beta(a) = \frac{\sqrt{\pi}}{2^{\frac{2a+1}{4}}\Gamma(\frac{a}{2}+\frac{3}{4})]}. \qquad (18)$$

Therefore, as $E \to \pm 0$, from Eq. (16), one gets: $\langle E_k^{a-\frac{1}{2}}\rangle_{KIM} \to 0$.

Thus, in this case, one gets

$$\langle E_k^{a-\frac{1}{2}}\rangle_{KIM} \cong E^{a-\frac{1}{2}}. \quad (19)$$

Second case: n-type-case ($E \leq 0$) and p-type-case ($E \geq 0$)

As $E \to \mp 0$, one has: $(y, \nu_{n(p)}) \to \pm 0$, and by putting $f(a) \equiv \frac{\eta_{n(p)}^{a-\frac{1}{2}}}{\sqrt{2\pi}} \times \Gamma(a+\frac{1}{2}) \times \beta(a)$, Eq. (18) yields

$$H_{n(p)}(\nu_{n(p)} \to \pm 0, N, r_{d(a)}, x, a) = \frac{(E_k^{a-\frac{1}{2}})_{KIM}}{f(a)} = \exp\left[-\frac{\mathcal{H}_{n(p)} \times R_{sn(cp)} \times (2a-1)}{8 \times \sqrt{|\nu_{n(p)}|}} - \left(\sqrt{a} + \frac{1}{16\sqrt{2}}\right) y - \left(\frac{1}{4} + \frac{1}{16a}\right) y^2 - \frac{y^3}{24\sqrt{a}}\right] \to 0. \quad (20)$$

Further, as $E \to \mp\infty$, one has: $(y, \nu_{n(p)}) \to \pm\infty$. Thus, one gets: $D_{-a-\frac{1}{2}}(y \to \pm\infty) \approx y^{-a-\frac{1}{2}} \times e^{-\frac{y^2}{4}} \to 0$.

Therefore, from Eq. (16), one gets

$$K_{n(p)}(\nu_{n(p)} \to \pm\infty, N, r_{d(a)}, x, a) \equiv \frac{(E_k^{a-\frac{1}{2}})_{KIM}}{f(a)} \simeq \frac{1}{\beta(a)} \times \exp\left(-\frac{(A_{n(p)} \times \nu_{n(p)})^2}{2}\right) \times (A_{n(p)} \times \nu_{n(p)})^{-a-\frac{1}{2}} \to 0, \quad (21)$$

noting that $\beta(a) = \frac{\sqrt{\pi}}{2^{\frac{2a+1}{4}} \Gamma(\frac{a}{2}+\frac{3}{4})]}$, being equal to: $\frac{\sqrt{\pi}}{2^{\frac{3}{4}} \times \Gamma(5/4)}$ for a=1, and $\frac{\sqrt{\pi}}{2^{3/2}}$ for $a = 5/2$.

It should be noted that those ratios: $\frac{(E_k^{a-\frac{1}{2}})_{KIM}}{f(a)}$, obtained in Equations (20) and (21), can be taken in an approximate form as

$$F_{n(p)}(\nu_{n(p)}, N, r_{d(a)}, x, a) = K_{n(p)}(\nu_{n(p)}, N, r_{d(a)}, x, a) + [H_{n(p)}(\nu_{n(p)}, N, r_{d(a)}, x, a) - K_{n(p)}(\nu_{n(p)}, N, r_{d(a)}, x, a)] \times \exp[-c_1 \times (A_{n(p)} \nu_{n(p)})^{c_2}],$$

so that: $F_{n(p)}(\nu_{n(p)}, N, r_{d(a)}, x, a) \to H_{n(p)}(\nu_{n(p)}, N, r_{d(a)}, x, a)$ for $0 \leq \nu_n \leq 16$, and $F_{n(p)}(\nu_{n(p)}, N, r_{d(a)}, x, a) \to K_{n(p)}(\nu_{n(p)}, N, r_{d(a)}, x, a)$ for $\nu_{n(p)} \geq 16$. Here, the constants c_1 and c_2 may be respectively chosen as: $c_1 = 10^{-40}$ and $c_2 = 80$, as $a = 1$, being used to determine the critical density of electrons (holes) localized in the exponential conduction(valence) band-tails (EBT), $N_{CDn(CDp)}^{EBT}(N, r_{d(a)}, x)$, given in the following.

Here, by using Eq. (18) for a=1, the density of states $\mathcal{D}(E)$ is defined by:

$$\langle \mathcal{D}(E_k) \rangle_{KIM} \equiv \frac{1}{2\pi^2}\left(\frac{2m_{c(v)}}{\hbar^2}\right)^{\frac{3}{2}} \times \langle E_k^{\frac{1}{2}} \rangle_{KIM} = \frac{1}{2\pi^2}\left(\frac{2m_{c(v)}}{\hbar^2}\right)^{\frac{3}{2}} \times \frac{\exp\left(-\frac{y^2}{4}\right) \times W_n^{\frac{1}{4}}}{\sqrt{2\pi}} \times \Gamma\left(\frac{3}{2}\right) \times D_{-\frac{3}{2}}(y) = \mathcal{D}(E). \quad (23)$$

Going back to the functions: H_n, K_n and F_n, given respectively in Equations (20-22), in which the factor $\frac{(E_k^{\frac{1}{2}})_{KIM}}{f(a=1)}$ is now replaced by

$$\frac{(E_g^{\frac{1}{2}})_{KIM}}{f(a=1)} = \frac{\mathcal{D}(E\leq 0)}{\mathcal{D}_o} = F_{n(p)}\left(\nu_{n(p)}, N, r_{d(a)}, x, a=1\right),\ \mathcal{D}_o(N, r_{d(a)}, x, a=1) = \frac{\left(m_{c(v)}\times m_o\right)^{3/2}\times\sqrt{\eta_{n(p)}}}{2\pi^2\hbar^3}\times\beta(a),$$

$$\beta(a=1) = \frac{\sqrt{\pi}}{2^{\frac{3}{4}}\times\Gamma(5/4)}. \qquad (24)$$

Therefore, $N^{EBT}_{CDn(CDp)}(N, r_{d(a)}, x)$ can be defined by: $N^{EBT}_{CDn(CDp)}(N, r_{d(a)}, x) = \int_{-\infty}^{U}\mathcal{D}(E\leq 0)\,dE$,

$$N^{EBT}_{CDn(CDp)}(N, r_{d(a)}, x) = \frac{\left(m_{c(v)}\right)^{3/2}\sqrt{\eta_{n(p)}}\times(\pm E_{Fn(Fp)})}{2\pi^2\hbar^3}\times\left\{\int_0^{16}\beta(a=1)\times F_{n(p)}\left(\nu_{n(p)}, N, r_{d(a)}, x, a=1\right)d\nu_{n(p)} + I_{n(p)}\right\}, \quad (25)$$

where

$$I_{n(p)} \equiv \int_{16}^{\infty}\beta(a=1)\times K_{n(p)}\left(\nu_{n(p)}, N, r_{d(a)}, x, a=1\right)d\nu_{n(p)} = \int_{16}^{\infty} e^{\frac{-\left(A_{n(p)}\times\nu_{n(p)}\right)^2}{2}}\times\left(A_{n(p)}\nu_{n(p)}\right)^{-3/2}d\nu_{n(p)}.$$

Then, by another variable change: $t = \left[A_{n(p)}\nu_{n(p)}/\sqrt{2}\right]^2$, the integral $I_{n(p)}$ yields

$I_{n(p)} = \frac{1}{2^{5/4}A_{n(p)}}\times\int_{z_{n(p)}}^{\infty} t^{b-1}e^{-t}dt \equiv \frac{\Gamma(b, z_{n(p)})}{2^{5/4}\times A_{n(p)}}$, where $b = -1/4$, $z_{n(p)} = \left[16A_{n(p)}/\sqrt{2}\right]^2$, and $\Gamma(b,\ z_{n(p)})$ is the incomplete Gamma function, defined by: $\Gamma(b, z_{n(p)}) \backsimeq z_{n(p)}^{b-1}\times e^{-z_{n(p)}}\left[1 + \sum_{j=1}^{16}\frac{(b-1)(b-2)\ldots(b-j)}{z_{n(p)}^{j}}\right]$.

Finally, Eq. (25) now yields

$$N^{EBT}_{CDn(CDp)}[N = N_{CDn(NDp)}(r_{d(a)}, x), r_{d(a)}, x] = \frac{\left(m_{c(v)}\right)^{3/2}\sqrt{\eta_{n(p)}}\times(\pm E_{Fn(Fp)})}{2\pi^2\hbar^3}\times\left\{\int_0^{16}\beta(a=1)\times F_{n(p)}\left(\nu_{n(p)}, N, r_{d(a)}, x, a=1\right)d\nu_{n(p)} + \frac{\Gamma(b, z_{n(p)})}{2^{5/4}\times A_{n(p)}}\right\}, \quad (26)$$

Being the density of electrons (holes) localized in the EBT, respectively.

In n(p)-type degenerate X(x) - crystalline alloys, the numerical results of $N^{EBT}_{CDn(CDp)}[N = N_{CDn(NDp)}(r_{d(a)}, x), r_{d(a)}, x] \equiv N^{EBT}_{CDn(CDp)}(r_{d(a)}, x)$, for a simplicity of presentation, evaluated using Eq. (26), are given in following Tables 1n and 1p in Appendix 1, in which those of other functions such as: $B_{do(ao)}$, ε, $E_{gno(gpo)}$, $N_{CDn(CDp)}$, and $N^{EBT}_{CDn(CDp)}$ are computed, using Equations (2), (5), (6), (8) and (26), respectively, noting that the relative deviations in absolute values are defined by: $|RD| \equiv \left|1 - \frac{N^{EBT}_{CDn(CDp)}}{N_{CDn(CDp)}}\right|$, giving rise to the maximal values of $|RD|$: $|RD|_{Max}(= 2.89\times10^{-7}$ and $2.88\times10^{-7})$, respectively.

Tables 1n and 1p in Appendix 1.

Table 1n. The numerical results of B_{do}, ε, E_{gno}, N_{CDn}, and N_{CDn}^{EBT} are computed, using Equations (2), (5), (6), (8), and (26), respectively, noting that the relative deviations in absolute values are defined by: $|RD| \equiv \left|1 - \frac{N_{CDn}^{EBT}}{N_{CDn}}\right|$, giving rise to a maximal value of $|RD|_{Max} (= \mathbf{2.89 \times 10^{-7}})$. Here, the value of the effective reduced Wigner-Seitz radius, obtained in Eq. (9a): at $N = N_{CDn}(r_d, x)$, $r_{sn}(N_{CDn}(r_d, x), r_d, x) =$ 2.4852548. Further, we obtain, at x=0 and $r_d = r_p$: $N_{CDn}^{EBT}(r_d, x) = 3.5201415 \times 10^{18}\ cm^{-3}$, in good accordance with that ($=3.52 \times 10^{18}\ cm^{-3}$), observed in the n-type Si-crystal [10, 11], and at x=1 and $r_d = r_p$: $N_{CDn}^{EBT}(r_d, x) = 4.3840013 \times 10^{16}\ cm^{-3}$, being higher than that ($=4.038 \times 10^{16}\ cm^{-3}$), given in the n-type Ge-crystal [12].

Donor	P	**Si**
r_d (nm) ↗	0.110	$\mathbf{r_{do}}$**=0.117**
x ↗	0, 0.5, 1	0, 0.5, 1
$B_{do}(x)$ in 10^{28} (N/m²) ↘		9.334069, 4.3327235, 1.5610697
$\varepsilon(r_d, x)$ ↘	11.58254, 13.81777, 16.052996	**11.4**, 13.6, **15.8**
$E_{gno}(r_d, x)$ eV ↗	1.168778, 0.955033, 0.7409956	**1.17**, 0.9556, **0.7412**
$N_{CDn}(r_d, x)$ in 10^{18} cm^{-3} ↗	3.5201424, 0.59776747, 0.043840025	3.6919625, 0.62694484, 0.045979882
$N_{CDn}^{EBT}(r_d, x)$ in 10^{18} cm^{-3} ↗	3.5201415, 0.59776731, 0.043840013	3.6919615, 0.62694467, 0.045979870
|RD| in 10^{-7}	2.69, 2.73, 2.65	2.65, 2.67, 2.70
$r_{sn}(N_{CDn}(r_d, x), r_d, x)$	2.4852548, 2.4852548, 2.4852548	2.4852548, 2.4852548, 2.4852548
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_d, x)$ ↘	10.165683, 12.12748, 14.089280	9.6901858, 11.56022, 13.4302575
$E_{gno}(r_d, x)$ eV ↗	1.1800687, 0.960274, 0.7428839	1.1850114, 0.962568, 0.7437106
$N_{CDn}(r_d, x)$ in 10^{18} cm^{-3} ↗	5.2066951, 0.88416678, 0.064844435	6.0113986, 1.0208163, 0.074866253
$N_{CDn}^{EBT}(r_d, x)$ in 10^{18} cm^{-3} ↗	5.2066937, 0.88416655, 0.064844418	6.0113970, 1.0208160, 0.074866233
|RD| in 10^{-7}	2.65, 2.65, 2.66	2.70, **2.89**, 2.74
$r_{sn}(N = N_{CDn}^{EBT}, r_d, x)$	2.4852548, 2.4852548, 2.4852548	2.4852548, 2.4852548, 2.4852548

Table 1p. The numerical results of B_{ao}, ε, E_{gpo}, N_{CDp}, and N_{CDp}^{EBT} are computed, using Equations (2), (5), (6), (8), and (26), respectively, noting that the relative deviations in absolute values are defined by: $|RD| \equiv \left|1 - \frac{N_{CDp}^{EBT}}{N_{CDp}}\right|$, giving rise to a maximal value of $|RD|_{Max} (= \mathbf{2.88 \times 10^{-7}})$. Here, the value of the effective reduced Wigner-Seitz radius, obtained in Eq. (9a): at $N = N_{CDp}(r_a, x)$, $r_{sn}(N_{CDp}(r_a, x), r_a, x) =$ 2.4852548. Further, we obtain, at x=0 and $r_a = r_B$: $N_{CDp}^{EBT}(r_a, x) = 4.0602418 \times 10^{18}\ cm^{-3}$, in good accordance

with that (=$4.06 \times 10^{18}\ cm^{-3}$), observed in the p-type Si-crystal [10, 11], and at x=1 and $r_a = r_B$: $N_{CDp}^{EBT}(r_a, x) = 2.6095232 \times 10^{17}\ cm^{-3}$, being higher than that (=$1.7347 \times 10^{17}\ cm^{-3}$), given in the p-type Ge-crystal [12].

Acceptor	B	**Si**
r_a (nm) ↗	0.088	**r_{a0}=0.117**
x ↗	0, 0.5, 1	0, 0.5, 1
$B_{ao}(x)$ in 10^9 (N/m²) ↘		13.50345, 7.377736, 3.902674
$\varepsilon(r_a,x)$ ↘	15.9777, 19.0611, 22.1445	**11.4**, 13.6, **15.8**
$E_{gpo}(r_a,x)$ eV ↗	1.14224, 0.94043, 0.73318	**1.17**, 0.9556, **0.7412**
$N_{CDp}(r_a,x)$ in 10^{18} cm^{-3} ↗	4.0602429, 1.1243180, 0.26095239	11.178374, 3.0953929, 0.71843565
$N_{CDp}^{EBT}(r_a,x)$ in 10^{18} cm^{-3} ↗	4.0602418, 1.1243177, 0.26095232	11.178371, 3.0953921, 0.71843546
|RD| in 10^{-7}	2.76, 2.47, 2.77	**2.88**, 2.62, 2.64
$r_{ap}(N = N_{CDp}^{EBT}, r_a, x)$	2.4852548, 2.4852548, 2.4852548	2.4852548, 2.4852548, 2.4852548
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_a,x)$ ↘	9.191081, 10.9648, 12.73851	8.687132, 10.36360, 12.0401
$E_{gpo}(r_a,x)$ eV ↗	1.200448, 0.97223, 0.749999	1.210834, 0.97791, 0.75300
$N_{CDp}(r_a,x)$ in 10^{18} cm^{-3} ↗	21.330127, 5.9065055, 1.3708903	25.261773, 6.9952139, 1.6235777
$N_{CDp}^{EBT}(r_a,x)$ in 10^{18} cm^{-3} ↗	21.330122, 5.9065040, 1.3708899	25.261767, 6.9952120, 1.6235773
|RD| in 10^{-7}	2.55, 2.61, 2.60	2.55, 2.67, 2.55
$r_{ap}(N = N_{CDp}^{EBT}, r_a, x)$	2.4852548, 2.4852548, 2.4852548	2.4852548, 2.4852548, 2.4852548

Thus, $\mathbf{N_{CDn(NDp)}}$, **determined in Eq. (8), is just** $\mathbf{N_{CDn(CDp)}^{EBT}}$, **given in Eq. (26), being the density of electrons (holes) localized in the EBT, respectively.** This is a new result.

Finally, the effective density of free electrons (holes), N^*, given in the parabolic conduction (valence) band of the n(p)-type degenerate $Si_{1-x}Ge_x$- crystalline alloy, can thus be expressed by $N^* \equiv N - N_{CDn(NDp)} \cong N - N_{CDn(CDp)}^{EBT}$. (27)

Optical band gap

Here, the optical band gap (**OBG**), $E_{gn1(gp1)}(N^*, r_{d(a)}, x, T)$, is defined by (Van Cong, 2024; 2023)

$$E_{gn1(gp1)}(N^*, r_{d(a)}, x, T) \equiv E_{gn2(gp2)}(N^*, r_{d(a)}, x, T) \pm E_{Fn(Fp)}(N^*, x, T),$$

$$E_{gn2(gp2)}(N^*, r_{d(a)}, x, T) \equiv E_{gno(gpo)}(r_{d(a)}, x) - \Delta T(T) - \Delta E_{gn(gp)}(N^*, r_{d(a)}, x), \quad (28)$$

where $E_{gn2(gp2)}$ is the reduced band gap, meaning that the band gap $E_{gno(gpo)}$, given in Equations (5, 6), is reduced by the effect of temperature, $\Delta T(T)$, being given in next Eq. (30), and that of high doping, $\Delta E_{gn(gp)}(N^*, r_{d(a)}, x)$, being determined in next Equations (31n, 31p), and finally, $\pm E_{Fn(Fp)}(N^*, x, T)$ is the Fermi energy, being determined in next Eq. (32). Then, it should be noted that, in the calculation of $\Delta E_{gn(gp)}$ and $E_{Fn(Fp)}$, the effective mass $m_{c(v)}(x)$ is now replaced by the reduced mass $m_r(x)$. Further, the reduced effective Wigner-Seitz radius, $r_{sn(sp)}$, characteristic of interactions, determined in Eq. (9a), and the Fermi wave number, $k_{Fn(Fp)}$, are now replaced by:

$$r_{sn(sp)}(N^*, r_{d(a)}, x) \equiv 1.1723 \times 10^8 \times \left(\frac{g_{c(v)}(x)}{N^*}\right)^{1/3} \times \frac{m_r(x)/m_o}{\varepsilon(r_{d(a)}, x)}, \; k_{Fn(Fp)}(N^*, r_{d(a)}, x) \equiv \left(3\pi^2 N^*/g_{c(v)}(x)\right)^{1/3}. \quad (29)$$

Here, in the n(p)-type degenerate X(x)$\equiv [Si_{1-x}(Ge_x)]$ crystalline alloy, $0 \leq x \leq 1$, the effective average number of equivalent conduction (valence)-band edges is determined by $g_c(x) = 4 \times x + 6 \times (1 - x)$, $g_v(x) = 2 \times x + 2 \times (1 - x)$.

Now, the expressions of ΔT, $\Delta E_{gn(gp)}$ and $\pm E_{Fn(Fp)}$ are determined in the following.

$\Delta T(T)$-Determination

Here, we have

$$\Delta T(T) = 10^{-4} \times T^2 \times \left[\frac{3.525 \times x}{T + 94\ K} + \frac{2.54 \times (1-x)}{T + 204\ K}\right]. \quad (30)$$

$\Delta E_{gn(gp)}(N^*, r_{d(a)}, x)$ –Determination

Then, the band gap narrowing $\Delta E_{gn}(N^*, x, T)$ is found to be given by

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

$$N_r \equiv \left(\frac{N^*}{N_{CDn}}\right), \quad (31n)$$

where $a_1 = 4.492098 \times 10^{-3}(eV)$, $a_2 = 7.6875582 \times 10^{-4}(eV)$, $a_3 = 3.3114218 \times 10^{-3}(eV)$, $a_4 = 6.64704 \times 10^{-3}(eV)$ and $a_5 = 9.5796678 \times 10^{-4}(eV)$, and

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

$$N_r \equiv \left(\frac{N^*}{N_{CDp}}\right), \quad (31p)$$

where $a_1 = 0.0183654\,(eV)$, $a_2 = 3.14145 \times 10^{-3}(eV)$, $a_3 = 0.014064\,(eV)$, $a_4 = 0.0270503\,(eV)$ and $a_5 = 3.91473 \times 10^{-3}(eV)$.

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

$$E_{cn(cp)}(N^*, r_{d(a)}, x) = \frac{-0.87553}{0.0908 + r_{sn(sp)}} + \frac{\frac{0.87553}{0.0908 + r_{sn(sp)}} + \left(\frac{2[1-\ln(2)]}{\pi^2}\right) \times \ln(r_{sn(sp)}) - 0.093288}{1 + 0.03847728 \times r_{sn(sp)}^{1.67878876}},$$

and $r_{sn(sp)}$ is determined in Eq. (29).

It should be noted in Equations (31n) and (31p) that, for given $r_{d(a)}$ and x, the values of $\Delta E_{gn(gp)}$ increase with increasing N.

$\pm E_{Fn(Fp)}(N^*, x, T)$ −Determination

Here, as given in our previous work,[8] for the n(p)-type, the Fermi energy $\pm E_{Fn(Fp)}$ was investigated, with a precision of the order of 2.11×10^{-4}, as:

$$\frac{E_{Fn}(u)}{k_B T}\left(\frac{-E_{Fp}(u)}{k_B T}\right) = \frac{G(u) + Au^B F(u)}{1 + Au^B},\ A = 0.0005372 \text{ and } B = 4.82842262, \qquad (32)$$

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

$N_{c(v)}(T,x) = 2 \times g_{c(v)}(x) \times \left(\frac{m_r(x) \times k_B T}{2\pi\hbar^2}\right)^{\frac{3}{2}}\ (cm^{-3})$, $F(u) = au^{\frac{2}{3}}\left(1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}}\right)^{-\frac{2}{3}}$,

$a = \left[(3\sqrt{\pi}/4) \times u\right]^{2/3}$, $b = \frac{1}{8}\left(\frac{\pi}{3}\right)^2$, $c = \frac{62.3739855}{1920}\left(\frac{\pi}{3}\right)^4$, and $G(u) \simeq \mathrm{Ln}(u) + 2^{-\frac{3}{2}} \times u \times e^{-du}$;

$d = 2^{3/2}\left[\frac{1}{\sqrt{27}} - \frac{3}{16}\right] > 0.$

Here, one notes that

(i) as $u \gg 1$, according to the degenerate case, Eq. (32) is reduced to the function F(u),

(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 non-degenerate case, Eq. (32) is reduced to the function G(u), and for given $r_{d(a)}$ and x, the values of $\pm E_{Fn(Fp)}$ increase with increasing N^*. *Now, going back to Eq. (28),*

(1)-the numerical results of $E_{gn1(gp1)}(N^*, r_{d(a)}, x = 0, T = 20\,K)$ are calculated, being in good agreement with experimental ones obtained by Wagner and del Alamo (1988), with maximal relative deviations: 5.38 % (9.07 %), and 2.06 % (5.16 %), as observed in the following Tables 2n and 2p in Appendix 1.

Tables 2n and 2p in Appendix 1

(2)-for $\mathbf{N} > N_{CDn(CDp)}(r_{d(a)}, x)$, the numerical results of the OBG, given in the n(p)-type, $E_{gn1}(N^*, r_{d(a)}, x, T = 20\,K)$, are obtained, using Eq. (28), as functions of N and $r_{d(a)}$, for x=0, 0.5, 1, respectively, being reported in following Tables 3n and 3p in Appendix 1.

Table 2n. Here, the numerical results of the optical band gap, given in the n(p)-type, $E_{gn1}(N^*, r_d = r_p, x = 0, T)$, expressed in eV, are obtained by using Eq. (28), respectively, noting that the maximal values of $\left|\mathbf{RD} = \mathbf{1} - \frac{E_{gn1}}{E_{gn1}^{Exp.}}\right|$, $E_{gn1}^{Exp.}$ being the experimental values given by Wagner and del Alamo (1988), are found to be given respectively, at T=20 K and T=300 K, by: 5.38 % (9.07 %).

N in 10^{18} cm^{-3}	4	8.5	15	50	80	150
$E_{gn1}^{Exp.}(N^*, r_p, 20K)$	1.138	1.133	1.129	1.131	1.132	1.133
$E_{gn1}(N^*, r_p, x = 0, 20K)$	1.161	1.158	1.157	1.165	1.174	1.194
|RD| in %	2.07	2.21	2.52	3.04	3.70	**5.38**
N in 10^{18} cm^{-3}	4	8.5	15	50	80	150
$E_{gn1}^{Exp.}(N^*, r_p, 300K)$	1.020	1.028	1.033	1.050	1.056	1.059
$E_{gn1}(N^*, r_p, x = 0, 300K)$	1.024	1.071	1.085	1.113	1.131	1.155
|RD| in %	0.48	4.24	5.10	5.97	7.15	**9.07**

Table 2p. Here, the numerical results of the optical band gap, given in the n(p)-type, $E_{gp1}(N^*, r_a = r_B, x = 0, T)$, expressed in eV, are obtained by using Eq. (28), respectively, noting that the maximal values of $\left|\mathbf{RD} = \mathbf{1} - \frac{E_{gp1}}{E_{gp1}^{Exp.}}\right|$, $E_{gp1}^{Exp.}$ being the experimental values given by Wagner and del Alamo (1988), are found to be given respectively, at T=20 K and T=300 K, by: 2.06 % (5.16 %).

N in 10^{18} cm^{-3}	6.5	11	15	26	60	170	400
$E_{gn1}^{Exp.}(N^*, r_B, 20K)$	1.142	1.140	1.139	1.142	1.142	1.162	1.178
$E_{gn1}(N^*, r_B, x = 0, 20K)$	1.156	1.142	1.136	1.127	1.121	1.138	1.202
|RD| in %	1.26	0.23	0.23	1.29	1.87	2.05	**2.06**

N in 10^{18} cm^{-3}	6.5	11	15	26	60	170	400
$E_{gn1}^{Exp.}(N^*, r_B, 300K)$ V	1.036	1.044	1.048	1.051	1.062	1.086	1.102
$E_{gn1}(N^*, r_B, x = 0, 300K)$	1.077	1.079	1.078	1.081	1.081	1.095	1.158
|RD| in %	3.96	3.38	2.92	2.91	1.81	0.91	**5.16**

Tables 3n and 3p in Appendix 1

Finally, in this degenerate X(x)- crystalline alloy, as noted in Equations (31n), (31p) and (32), because both two functions: $\Delta E_{gn(gp)}$ and $\pm E_{Fn(Fp)}$, for given $r_{d(a)}$ and x, increase with increasing N^*, $E_{gn1}(N^*, r_{d(a)}, x, T = 20\,K)$, determined in Eq. (28), and expressed as functions of N^*, thus randomly varies.

Table 3n. Here, for $N > N_{CDn}(r_d, x)$, the numerical results of the optical band gap, $E_{gn1}(N^*, r_d, x, T = 20\ K)$, are obtained by using Eq. (28), as functions of N and r_d, for x=0, 0.5, 1, respectively. Here, for given N and r_d, E_{gn1} decreases with increasing x, since $E_{gno}(r_d, x)$ decreases, as observed in Table 1n.

N in 10^{18} cm^{-2}	4	8.5	15	50	80	150
x=0						
$E_{gn1}(N^*, r_p, x, T)$ in eV	1.161	1.158	1.157	1.165	1.174	1.194
$E_{gn1}(N^*, r_{Si}, x, T)$ in eV	1.161	1.157	1.156	1.164	1.173	1.194
$E_{gn1}(N^*, r_{Sb}, x, T)$ in eV		1.169	1.168	1.179	1.189	1.211
$E_{gn1}(N^*, r_{Sn}, x, T)$ in eV		1.174	1.173	1.185	1.195	1.219
x=0.5						
$E_{gn1}(N^*, r_p, x, T)$ in eV	0.924	0.917	0.911	0.905	0.908	0.920
$E_{gn1}(N^*, r_{Si}, x, T)$ in eV	0.924	0.917	0.912	0.906	0.909	0.923
$E_{gn1}(N^*, r_{Sb}, x, T)$ in eV	0.932	0.926	0.922	0.923	0.929	0.948
$E_{gn1}(N^*, r_{Sn}, x, T)$ in eV	0.936	0.930	0.927	0.929	0.937	0.958
x=1						
$E_{gn1}(N^*, r_p, x, T)$ in eV	0.616	0.576	0.539	0.438	0.392	0.327
$E_{gn1}(N^*, r_{Si}, x, T)$ in eV	0.617	0.578	0.542	0.445	0.400	0.339
$E_{gn1}(N^*, r_{Sb}, x, T)$ in eV	0.631	0.598	0.568	0.491	0.459	0.419
$E_{gn1}(N^*, r_{Sn}, x, T)$ in eV	0.637	0.605	0.578	0.509	0.482	0.450

Table 3p. Here, for $N > N_{CDp}(r_a, x)$, the numerical results of $E_{gp1}(N^*, r_a, x, T = 20\ K)$, are obtained by using Eq. (28), as functions of N and r_a , for x=0, 0.5, 1, respectively. Here, for given N and r_a, E_{gp1} decreases with increasing x, since $E_{gpo}(r_a, x)$ decreases, as observed in Table 1p.

N in 10^{18} cm^{-3}	6.5	11	15	26	60	170	400
x=0							
$E_{gp1}(N^*, r_B, T)$ in eV	1.156	1.142	1.136	1.127	1.121	1.138	1.202
$E_{gp1}(N^*, r_{Si}, T)$ in eV			1.132	1.125	1.133	1.183	1.291
$E_{gp1}(N^*, r_{In}, T]$ in eV				1.165	1.175	1.241	1.371
$E_{gp1}(N^*, r_{Cd}, T]$ in eV				1.186	1.186	1.256	1.391
x=0.5							
$E_{gp1}(N^*, r_B, T)$ in eV	0.872	0.851	0.838	0.814	0.777	0.744	0.759
$E_{gp1}(N^*, r_{Si}, T)$ in eV	0.889	0.874	0.866	0.855	0.848	0.879	0.977
$E_{gp1}(N^*, r_{In}, T]$ in eV	0.935	0.909	0.901	0.896	0.903	0.963	1.102
$E_{gp1}(N^*, r_{Cd}, T]$ in eV		0.919	0.912	0.906	0.916	0.983	1.131
x=1							
$E_{gp1}(N^*, r_B, T)$ in eV	0.549	0.507	0.480	0.427	0.336	0.227	0.185
$E_{gp1}(N^*, r_{Si}, T)$ in eV	0.601	0.578	0.564	0.541	0.516	0.539	0.673
$E_{gp1}(N^*, r_{In}, T]$ in eV	0.638	0.622	0.615	0.605	0.612	0.699	0.916
$E_{gp1}(N^*, r_{Cd}, T]$ in eV	0.647	0.633	0.627	0.621	0.634	0.735	0.971

CONCLUSION

In those Tables, some concluding remarks are given and discussed in the following.

(1)-For a given x, while $\varepsilon(r_{d(a)},x)$ decreases (↘), the functions: $E_{gno(gpo)}(r_{d(a)},x)$, $N_{CDn(CDp)}(r_{d(a)},x)$ and $N^{EBT}_{CDn(CDp)}(r_{d(a)},x)$ increase (↗), with increasing (↗) $r_{d(a)}$, due to the impurity size effect, as observed in Tables 1n and 1p in Appendix 1.

(2)-Further, for a given $r_{d(a)}$, while $\varepsilon(r_{d(a)},x)$ also decreases (↘), the functions: $E_{gno(gpo)}(r_{d(a)},x)$, $N_{CDn(CDp)}(r_{d(a)},x)$ and $N^{EBT}_{CDn(CDp)}(r_{d(a)},x)$ also increase (↗), with increasing (↗) x, as observed in Tables 1n and 1p in Appendix 1.

(3)- In those Tables 1n and 1p, one also notes that the maximal value of |RD| is found to be given by: 2.89×10^{-7}, meaning that $N^{EBT}_{CDn(CDp)} \cong N_{CDn(CDp)}$. In other words, such the critical d(a)-density $N_{CDn(NDp)}(r_{d(a))},x)$, is just the density of electrons (holes), localized in the EBT, $N^{EBT}_{CDn(CDp)}(r_{d(a)},x)$, respectively.

(4) Finally, once $N_{CDn(CDp)}$ is determined, the effective density of free electrons (holes), N^*, given in the parabolic conduction (valence) band of the n(p)-type degenerate $X(x)$- crystalline alloy, can thus be defined, as those defined in the compensated crystals, by:

$$N^*(N, r_{d(a)}, x) \equiv N - N_{CDn(NDp)} \cong N - N^{EBT}_{CDn(CDp)},$$

Needing to determine the optical, electrical, and thermoelectric properties in such n(p)-type degenerate X(x)-crystalline alloys, as those studied in n(p)-type degenerate crystals [3-12].

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Appendix 1

Table 1: The numerical results of B_{do}, ε, E_{gno}, N_{CDn}, and N_{CDn}^{EBT} are computed, using Equations (2), (5), (6), (8), and (26), respectively, noting that the relative deviations in absolute values are defined by: $|RD| \equiv \left|1-\frac{N_{CDn}^{EBT}}{N_{CDn}}\right|$, giving rise to a maximal value of $|RD|_{Max}(=2.89\times10^{-7})$. Here, the value of the effective reduced Wigner-Seitz radius, obtained in Eq. (9a): at $N = N_{CDn}(r_d,x)$, $r_{an}(N_{CDn}(r_d,x),r_d,x) =$ 2.4852548. Further, we obtain, at x=0 and $r_d = r_p$: $N_{CDn}^{EBT}(r_d,x) = 3.5201415\times10^{18}\ cm^{-2}$, in good accordance with that ($=3.52\times10^{18}\ cm^{-2}$), observed in the n-type Si-crystal [10, 11], and at x=1 and $r_d = r_p$: $N_{CDn}^{EBT}(r_d,x) = 4.3840013\times10^{18}\ cm^{-2}$, being higher than that ($=4.038\times10^{18}\ cm^{-2}$), given in the n-type Ge-crystal.[12]

Donor	P	**Si**
r_d (nm) ↗	0.110	**r_{do}=0.117**
x ↗	0, 0.5, 1	0, 0.5, 1
$B_{do}(x)$ in 10^{8} (N/m^2) ↘		9.334069, 4.3327235, 1.5610697
$\varepsilon(r_d,x)$ ↘	11.58254, 13.81777, 16.052996	**11.4**, 13.6, **15.8**
$E_{gno}(r_d,x)$ eV ↗	1.168778, 0.955033, 0.7409956	**1.17**, 0.9556, **0.7412**
$N_{CDn}(r_d,x)$ in 10^{18} cm^{-2} ↗	3.5201424, 0.59776747, 0.043840025	3.6919625, 0.62694484, 0.045979882
$N_{CDn}^{EBT}(r_d,x)$ in 10^{18} cm^{-2} ↗	3.5201415, 0.59776731, 0.043840013	3.6919615, 0.62694467, 0.045979870
$\|RD\|$ in 10^{-7}	2.69, 2.73, 2.65	2.65, 2.67, 2.70
$r_{an}(N_{CDn}(r_d,x),r_d,x)$	2.4852548, 2.4852548, 2.4852548	2.4852548, 2.4852548, 2.4852548

Donor	Sb	Sn
r_d (nm) ↗	0.136	0.140
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_d,x)$ ↘	10.165683, 12.12748, 14.089280	9.6901858, 11.56022, 13.4302575
$E_{gno}(r_d,x)$ eV ↗	1.1800687, 0.960274, 0.7428839	1.1850114, 0.962568, 0.7437106
$N_{CDn}(r_d,x)$ in 10^{18} cm^{-2} ↗	5.2066951, 0.88416678, 0.064844435	6.0113986, 1.0208163, 0.074866253
$N_{CDn}^{EBT}(r_d,x)$ in 10^{18} cm^{-2} ↗	5.2066937, 0.88416655, 0.064844418	6.0113970, 1.0208160, 0.074866233
$\|RD\|$ in 10^{-7}	2.65, 2.65, 2.66	2.70, **2.89**, 2.74
$r_{an}(N = N_{CDn}^{EBT},r_d,x)$	2.4852548, 2.4852548, 2.4852548	2.4852548, 2.4852548, 2.4852548

Table 1p: The numerical results of B_{ao}, ε, E_{gpo}, N_{CDp}, and N_{CDp}^{EBT} are computed, using Equations (2), (5), (6), (8), and (26), respectively, noting that the relative deviations in absolute values are defined by: $|RD| \equiv \left|1-\frac{N_{CDp}^{EBT}}{N_{CDp}}\right|$, giving rise to a maximal value of $|RD|_{Max}(=2.88\times10^{-7})$. Here, the value of the effective reduced Wigner-Seitz radius, obtained in Eq. (9a): at $N = N_{CDp}(r_a,x)$, $r_{an}(N_{CDp}(r_a,x),r_a,x) =$ 2.4852548. Further, we obtain, at x=0 and $r_a = r_B$: $N_{CDp}^{EBT}(r_a,x) = 4.0602418\times10^{18}\ cm^{-2}$, in good accordance with that ($=4.06\times10^{18}\ cm^{-2}$), observed in the p-type Si-crystal [10, 11], and at x=1 and $r_a = r_B$: $N_{CDp}^{EBT}(r_a,x) = 2.6095232\times10^{17}\ cm^{-2}$, being higher than that ($=1.7347\times10^{17}\ cm^{-2}$), given in the p-type Ge-crystal.[12]

Acceptor	B	**Si**
r_B (nm) ↗	0.088	**r_{ao}=0.117**
x ↗	0, 0.5, 1	0, 0.5, 1
$B_{ao}(x)$ in 10^{8} (N/m^2) ↘		13.50345, 7.377736, 3.902674
$\varepsilon(r_a,x)$ ↘	15.9777, 19.0611, 22.1445	**11.4**, 13.6, **15.8**

$E_{gp0}(r_a, x)$ eV ↗	1.14224, 0.94043, 0.73318	**1.17**, 0.9556, **0.7412**
$N_{CD_D}(r_a, x)$ in 10^{18} cm^{-2} ↗	4.0602429, 1.1243180, 0.26095239	11.178374, 3.0953929, 0.71843565
$N_{CD_D}^{EBT}(r_a, x)$ in 10^{18} cm^{-2} ↗	4.0602418**,** 1.1243177**,** 0.26095232	11.178371**,** 3.0953921**,** 0.71843546
$\|RD\|$ in 10^{-7}	2.76, 2.47, 2.77	**2.88**, 2.62, 2.64
$r_{ap}(N = N_{CD_D}^{EBT}, r_a, x)$	2.4852548, 2.4852548, 2.4852548	2.4852548, 2.4852548, 2.4852548
Acceptor	In	Cd
r_a (nm) ↗	0.144	0.148
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_a, x)$ ↘	9.191081, 10.9648, 12.73851	8.687132, 10.36360, 12.0401
$E_{gp0}(r_a, x)$ eV ↗	1.200448, 0.97223, 0.749999	1.210834, 0.97791, 0.75300
$N_{CD_D}(r_a, x)$ in 10^{18} cm^{-2} ↗	21.330127, 5.9065055, 1.3708903	25.261773, 6.9952139, 1.6235777
$N_{CD_D}^{EBT}(r_a, x)$ in 10^{18} cm^{-2} ↗	21.330122**,** 5.9065040**,** 1.3708899	25.261767**,** 6.9952120**,** 1.6235773
$\|RD\|$ in 10^{-7}	2.55, 2.61, 2.60	2.55, 2.67, 2.55
$r_{ap}(N = N_{CD_D}^{EBT}, r_a, x)$	2.4852548, 2.4852548, 2.4852548	2.4852548, 2.4852548, 2.4852548

Table 2: Here, the numerical results of the optical band gap, given in the n(p)-type, $E_{gn1}(N^*, r_d = r_p, x = 0, T)$, expressed in eV, are obtained by using Eq. (28), respectively, noting that the maximal values of $\left|RD = 1 - \frac{E_{gn1}}{E_{gn1}^{Exp.}}\right|$, $E_{gn1}^{Exp.}$ being the experimental values given by Wagner and del Alamo (1988), are found to be given respectively, at T=20 K and T=300 K, by: 5.38 % (9.07 %).

N in 10^{18} cm^{-2}	4	8.5	15	50	80	150
$E_{gn1}^{Exp.}(N^*, r_p, 20K)$	1.138	1.133	1.129	1.131	1.132	1.133
$E_{gn1}(N^*, r_p, x = 0, 20K)$	1.161	1.158	1.157	1.165	1.174	1.194
$\|RD\|$ in %	2.07	2.21	2.52	3.04	3.70	**5.38**

N in 10^{18} cm^{-2}	4	8.5	15	50	80	150
$E_{gn1}^{Exp.}(N^*, r_p, 300K)$	1.020	1.028	1.033	1.050	1.056	1.059
$E_{gn1}(N^*, r_p, x = 0, 300K)$	1.024	1.071	1.085	1.113	1.131	1.155
$\|RD\|$ in %	0.48	4.24	5.10	5.97	7.15	**9.07**

Table 2p: Here, the numerical results of the optical band gap, given in the n(p)-type, $E_{gp1}(N^*, r_a = r_B, x = 0, T)$, expressed in eV, are obtained by using Eq. (28), respectively, noting that the maximal values of $\left|RD = 1 - \frac{E_{gp1}}{E_{gp1}^{Exp.}}\right|$, $E_{gp1}^{Exp.}$ being the experimental values given by Wagner and del Alamo (1988), are found to be given respectively, at T=20 K and T=300 K, by: 2.06 % (5.16 %).

N in 10^{18} cm^{-2}	6.5	11	15	26	60	170	400
$E_{gp1}^{Exp.}(N^*, r_B, 20K)$	1.142	1.140	1.139	1.142	1.142	1.162	1.178
$E_{gp1}(N^*, r_B, x = 0, 20K)$	1.156	1.142	1.136	1.127	1.121	1.138	1.202

$\|RD\|$ in %	1.26	0.23	0.23	1.29	1.87	2.05	**2.06**
N in 10^{18} cm^{-3}	6.5	11	15	26	60	170	400
$E_{gp1}^{Exp.}(N^*, r_B, 300K)$ V	1.036	1.044	1.048	1.051	1.062	1.086	1.102
$E_{gp1}(N^*, r_B, x = 0, 300K)$	1.077	1.079	1.078	1.081	1.081	1.095	1.158
$\|RD\|$ in %	3.96	3.38	2.92	2.91	1.81	0.91	**5.16**

Table 3n: Here, for $N > N_{CDn}(r_d, x)$, the numerical results of the optical band gap, $E_{gn1}(N^*, r_d, x, T = 20\,K)$, are obtained by using Eq. (28), as functions of N and r_d, for x=0, 0.5, 1, respectively. Here, for given N and r_d, E_{gn1} decreases with increasing x, since $E_{gno}(r_d, x)$ decreases, as observed in Table 1n.

N in 10^{18} cm^{-3}	4	8.5	15	50	80	150
x=0						
$E_{gn1}(N^*, r_p, x, T)$ in eV	1.161	1.158	1.157	1.165	1.174	1.194
$E_{gn1}(N^*, r_{Si}, x, T)$ in eV	1.161	1.157	1.156	1.164	1.173	1.194
$E_{gn1}(N^*, r_{Sb}, x, T)$ in eV		1.169	1.168	1.179	1.189	1.211
$E_{gn1}(N^*, r_{Sn}, x, T)$ in eV		1.174	1.173	1.185	1.195	1.219
x=0.5						
$E_{gn1}(N^*, r_p, x, T)$ in eV	0.924	0.917	0.911	0.905	0.908	0.920
$E_{gn1}(N^*, r_{Si}, x, T)$ in eV	0.924	0.917	0.912	0.906	0.909	0.923
$E_{gn1}(N^*, r_{Sb}, x, T)$ in eV	0.932	0.926	0.922	0.923	0.929	0.948
$E_{gn1}(N^*, r_{Sn}, x, T)$ in eV	0.936	0.930	0.927	0.929	0.937	0.958
x=1						
$E_{gn1}(N^*, r_p, x, T)$ in eV	0.616	0.576	0.539	0.438	0.392	0.327
$E_{gn1}(N^*, r_{Si}, x, T)$ in eV	0.617	0.578	0.542	0.445	0.400	0.339
$E_{gn1}(N^*, r_{Sb}, x, T)$ in eV	0.631	0.598	0.568	0.491	0.459	0.419
$E_{gn1}(N^*, r_{Sn}, x, T)$ in eV	0.637	0.605	0.578	0.509	0.482	0.450

Table 3p: Here, for $N > N_{CDp}(r_a, x)$, the numerical results of $E_{gp1}(N^*, r_a, x, T = 20\,K)$, are obtained by using Eq. (28), as functions of N and r_a, for x=0, 0.5, 1, respectively. Here, for given N and r_a, E_{gp1} decreases with increasing x, since $E_{gpo}(r_a, x)$ decreases, as observed in Table 1p.

N in 10^{18} cm^{-3}	6.5	11	15	26	60	170	400
x=0							

$E_{gD1}(N^*, r_B, T)$ in eV	1.156		1.142	1.136		1.127		1.121	1.138	1.202
$E_{gD1}(N^*, r_{Si}, T)$ in eV			1.132		1.125		1.133	1.183	1.291	
$E_{gD1}(N^*, r_{In}, T)$ in eV				1.165		1.175	1.241	1.371		
$E_{gD1}(N^*, r_{Cd}, T)$ in eV				1.186		1.186	1.256	1.391		

x=0.5

$E_{gD1}(N^*, r_B, T)$ in eV	0.872		0.851	0.838	0.814		0.777	0.744	0.759	
$E_{gD1}(N^*, r_{Si}, T)$ in eV	0.889		0.874	0.866	0.855		0.848	0.879	0.977	
$E_{gD1}(N^*, r_{In}, T)$ in eV	0.935		0.909	0.901	0.896		0.903	0.963	1.102	
$E_{gD1}(N^*, r_{Cd}, T)$ in eV		0.919	0.912	0.906		0.916	0.983	1.131		

x=1

$E_{gD1}(N^*, r_B, T)$ in eV	0.549	0.507	0.480	0.427	0.336	0.227	0.185	
$E_{gD1}(N^*, r_{Si}, T)$ in eV	0.601	0.578	0.564	0.541	0.516	0.539	0.673	
$E_{gD1}(N^*, r_{In}, T)$ in eV	0.638	0.622	0.615	0.605	0.612	0.699	0.916	
$E_{gD1}(N^*, r_{Cd}, T)$ in eV	0.647	0.633	0.627	0.621	0.634	0.735	0.971	