



Same maximum figure of merit $ZT(=1)$, due to effects of impurity size and heavy doping, obtained in the n(p)-type degenerate InP-crystal ($\xi_{n(p)}(\geq 1)$), at same reduced Fermi energy $\xi_{n(p)}(= 1.813)$ and same minimum (maximum) Seebeck coefficient $S_b(= (\mp)1.563 \times 10^{-4} \frac{V}{K})$, at which same

$$(ZT)_{\text{Mott}}(= \frac{\pi^2}{3 \times \xi_{n(p)}^2} \simeq 1)$$

H. 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.

Email: van-cong.huynh@univ-perp.fr ; huynhvc@outlook.fr

Abstract

In our two previous papers [1, 2], referred to as I and II. In I, our new expression for the extrinsic static dielectric constant, $\epsilon(r_{d(a)})$, $r_{d(a)}$ being the donor (acceptor) d(a)-radius, was determined by using an effective Bohr model, suggesting that, for an increasing $r_{d(a)}$, $\epsilon(r_{d(a)})$, due to such the impurity size effect, decreases, and affecting strongly the critical impurity density in the metal-insulator transition and also various majority carrier transport coefficients given in the n(p)-type degenerate InP-crystal, defined for the reduced Fermi energy $\xi_{n(p)}(\geq 1)$. Then, using the same physical model and same mathematical methods and taking into account the corrected values of energy-band-structure parameters, all the numerical results, obtained in II, are now revised and performed, giving rise to some important concluding remarks, as follows.

(1) The critical donor(acceptor)-density, $N_{CDn(NDp)}(r_{d(a)})$, determined in Eq. (3), can be explained by the densities of electrons (holes) localized in exponential conduction (valance)-band (EBT) tails, $N_{CDn(CDp)}^{EBT}(r_{d(a)})$, given in Eq. (21).

(2) In Tables 9-11, for a given d(a)-density $N [\geq 2N_{CDn(NDp)}(r_{d(a)})]$ one notes here that with increasing temperature T(K): **(i)** for reduced Fermi energy $\xi_{n(p)}(= 1.813)$, while the numerical results of the Seebeck coefficient S_b present a same minimum (maximum) $(= (\mp)1.563 \times 10^{-4} \frac{V}{K})$, those of the figure of merit ZT show a same maximum $ZT(= 1)$, **(ii)** for $\xi_n = 1$, those of S_b and ZT present same results:

Sb ($= (\mp)1.322 \times 10^{-4} \frac{V}{K}$) and 0.715, respectively, **(iii)** for $\xi_{n(p)} = 1.813$ and $\xi_{n(p)} = 1$, those of the well-known Mott figure of merit give same $(ZT)_{\text{Mott}} = \frac{\pi^2}{3 \times \xi_{n(p)}^2} (\simeq 1 \text{ and } 3.290)$, respectively, and finally, **(iv)** we show here that in the degenerate InP-semiconductor, the Wiedemann-Frank law, given in Eq. (25a), is found to be exact.

Keywords: Effects of the impurity-size and heavy doping; effective autocorrelation function for potential fluctuations; optical, electrical, and thermoelectric properties; figure of merit; Wiedemann-Franz law

1. Introduction

In our two previous papers [1, 2], referred here to as I and II.

In I, our new expression for the extrinsic static dielectric constant, $\varepsilon(r_{d(a)})$, $r_{d(a)}$ being the donor (acceptor) d(a)-radius, was determined by using an effective Bohr model, suggesting that, for an increasing $r_{d(a)}$, $\varepsilon(r_{d(a)})$, due to such the impurity size effect, decreases, and affecting strongly the critical impurity density in the metal-insulator transition and also various majority carrier-transport coefficients given in n(p)-type degenerate InP-crystal, defined for the accurate reduced Fermi energy [3], $\xi_{n(p)} (\geq 1)$. Therefore, all the numerical results of those obtained and given in II are now revised and performed, in comparison with those obtained in [3-11].

In Section 2, the numerical results of energy-band-structure parameters [4, 5, 6] are presented in Tables 1 and 2. In Section 3, the values of optical band gap are given in Table 3. In Section 4, the physical and mathematical methods, needed to determine and evaluate the critical densities of the majority carriers localized in the exponential conduction (valence) band tails, are presented, confirming thus the corresponding numerical results, obtained using Eq. (3) for the generalized effective Mott criterion in the metal-insulator transition (**MIT**), as observed in Table 2. In Section 5, based on the Fermi-Dirac distribution function method, our accurate expression for the electrical conductivity, σ , is determined, being a fundamental one, since it is related to all other electrical-and-thermoelectric coefficients, and then all the numerical results of those coefficients are reported in Tables 4-11. Finally, some concluding remarks are given in Section 6.

2. Energy-band-structure parameters

First of all, we present in Table 1 the values of the energy-band-structure parameters, given in the n(p)-type InP-crystal, such as: (i) if denoting the free electron mass by m_0 , the relative effective electron (hole) mass, $m_{n(p)}^*/m_0$, which is equal to the relative effective mass, $m_{n(p)}/m_0$ [4], as used in this Sections 2 and 4 to determine the critical impurity density in the MIT, (ii) to the reduced effective mas, $m_r = \frac{m_n \times m_p}{m_n + m_p} \times m_0$, as used in Section 3 to determine the optical band gap (**OBG**), and (iii), to the conductivity effective mass,

$m_{\text{Cn(Cp)}}/m_0$ [5], as used in Section 5 to determine the electrical-and-thermoelectric coefficients. Further, $\mathbb{E}_{\text{go}} = \mathbb{E}_{\text{go}}(r_{\text{do(ao)}} = r_{\text{P(In)}}) = 1.424 \text{ eV}$ [5] is the unperturbed intrinsic band gap, as used in Section 3 to determine the OBG, $\epsilon_0 = 12.5$ [4], is the relative intrinsic dielectric constant, and finally, the effective averaged numbers of equivalent conduction (valence)-band edge, $g_{\text{c(v)}} = 1(1)$, used for present majority-carrier transport phenomena.

Table 1. Here, the effective electron (hole) mass, $m_{\text{n(p)}}^*$, is equal respectively to: $m_{\text{n(p)}}$, as used in Sections 2 and 4, to m_r in Section 3, and $m_{\text{Cn(Cp)}}$ in Section 5, and the values of other important parameters are also reported.

$m_{\text{n(p)}}/m_0$ [1]	m_r/m_0	$m_{\text{Cn(Cp)}}/m_0$ [5]	$g_{\text{c(v)}}$	\mathbb{E}_{go} [5]	ϵ_0 [4]
$0.073(\frac{0.078+0.6}{2} = 0.339)$	0.060	0.077(0.50)	1(1)	1.424 eV	12.5

We now determine our expression for extrinsic static dielectric constant, $\epsilon(r_{\text{d(a)}})$, due to the impurity size effect, and the expression for critical density, $N_{\text{CDn(CDp)}}(r_{\text{d(a)}})$, characteristic of the MIT, as follows.

2.1. Expression for $\epsilon(r_{\text{d(a)}})$

In the [d(a)-semiconductors]-systems, since $r_{\text{d(a)}}$, given in tetrahedral covalent bonds, is usually either larger or smaller than $r_{\text{do(ao)}} \equiv r_{\text{P(In)}}$, a local mechanical strain (or deformation potential energy) is induced, according to a compression (dilation) for: $r_{\text{d(a)}} > r_{\text{do(ao)}} (r_{\text{d(a)}} < r_{\text{do(ao)}})$, due to the d(a)-size effect, respectively [1]. Then, we have shown that this $r_{\text{d(a)}}$ -effect affects the changes in all the energy-band-structure parameters, expressed in terms of the static dielectric constant, $\epsilon(r_{\text{d(a)}})$, determined as follows.

At $T=0\text{K}$, we shown [1] that, as $r_{\text{d(a)}} > r_{\text{do(ao)}} (r_{\text{d(a)}} < r_{\text{do(ao)}})$, such the compression (dilatation) corresponding the repulsive (attractive) force increases (decreases) the intrinsic energy gap $\mathbb{E}_{\text{gni(gpi)}}(r_{\text{d(a)}})$ and the effective donor(acceptor)-ionization energy $\mathbb{E}_{\text{d(a)}}(r_{\text{d(a)}})$ in absolute values, obtained in an effective Bohr model, as [1]:

$$\mathbb{E}_{\text{gni(gpi)}}(r_{\text{d(a)}}) - \mathbb{E}_{\text{go}}(r_{\text{do(ao)}}) = \mathbb{E}_{\text{d(a)}}(r_{\text{d(a)}}) - \mathbb{E}_{\text{do(ao)}}(r_{\text{do(ao)}}) = \mathbb{E}_{\text{do(ao)}}(r_{\text{do(ao)}}) \times \left[\left(\frac{\epsilon_0}{\epsilon(r_{\text{d(a)}})} \right)^2 - 1 \right], \quad (1)$$

where

$$\epsilon(r_{\text{d(a)}}) = \frac{\epsilon_0}{\sqrt{1 + \left[\left(\frac{r_{\text{d(a)}}}{r_{\text{do(ao)}}} \right)^3 - 1 \right] \times \ln \left(\frac{r_{\text{d(a)}}}{r_{\text{do(ao)}}} \right)^3}} \leq \epsilon_0, \text{ for } r_{\text{d(a)}} \geq r_{\text{do(ao)}}, \text{ and}$$

$$\epsilon(r_{\text{d(a)}}) = \frac{\epsilon_0}{\sqrt{1 - \left[\left(\frac{r_{\text{d(a)}}}{r_{\text{do(ao)}}} \right)^3 - 1 \right] \times \ln \left(\frac{r_{\text{d(a)}}}{r_{\text{do(ao)}}} \right)^3}} \geq \epsilon_0, \left[\left(\frac{r_{\text{d(a)}}}{r_{\text{do(ao)}}} \right)^3 - 1 \right] \times \ln \left(\frac{r_{\text{d(a)}}}{r_{\text{do(ao)}}} \right)^3 < 1, \text{ for } r_{\text{d(a)}} \leq r_{\text{do(ao)}}. \quad (2)$$

One notes that $\epsilon(r_{\text{d(a)}})$ decreases with an increasing $r_{\text{d(a)}}$.

2.2. Our expressions for the critical density in the MIT

In the n(p)-type degenerate InP-semiconductor, the critical donor(acceptor)-density, $N_{\text{CDn(NDp)}}(r_{\text{d(a)}})$, is determined from the generalized effective Mott criterion in the MIT, as:

$$N_{\text{CDn(NDp)}}(r_{\text{d(a)}})^{1/3} \times a_{\text{Bn(Bp)}}(r_{\text{d(a)}}) = 0.25, \quad (3)$$

and the effective Bohr radius $a_{Bn(Bp)}(r_{d(a)})$ is given by:

$$a_{Bn(Bp)}(r_{d(a)}) \equiv \frac{\varepsilon(r_{d(a)}) \times \hbar^2}{(m_{n(p)}^*/m_0) \times q^2} = 0.53 \times 10^{-8} \text{ cm} \times \frac{\varepsilon(r_{d(a)})}{(m_{n(p)}^*/m_0)}, \quad (4)$$

where $-q$ is the electron charge, $\varepsilon(r_{d(a)})$ is determined in Eq. (2), and $m_{n(p)}^*/m_0 = m_{n(p)}/m_0 = 0.073(0.339)$, as given in Table 1. In this Table 2, we also present various values of $\varepsilon(r_{d(a)})$, $a_{Bn(Bp)}(r_{d(a)})$, $E_{d(a)}(r_{d(a)})$ and $E_{gni(gpi)}(r_{d(a)})$, $N_{CDn(NDp)}(r_{d(a)})$, and the densities of electrons (holes) localized in exponential conduction (valence)-band tails, $N_{CDn(CDp)}^{EBT}(r_{d(a)})$, noting that the maximal relative deviations, in absolute values, $|RD|$, between $N_{CDn(NDp)}(r_{d(a)})$ and $N_{CDn(CDp)}^{EBT}(r_{d(a)})$ are found to be equal to: $5.57(7.61) \times 10^{-4}$, respectively. In other word, $N_{CDn(NDp)}(r_{d(a)})$, determined in Eq. (3), can be explained by $N_{CDn(CDp)}^{EBT}(r_{d(a)})$, determined in Eq. (21). Furthermore, in our recent work [6], we showed that, in the n(p)-type degenerate semiconductors, the critical densities of electrons (holes) can also be determined from the spin-susceptibility singularities (SSS), obtained at $N = N_{CDn(CDp)}^{SSS}(r_{d(a)})$, at which the MITs occur.

Table 2. Here, for increasing $r_{d(a)}$ [4], both $\varepsilon(r_{d(a)})$, calculated using Eq. (2), and $a_{Bn(Bp)}(r_{d(a)})$, evaluated using Eq. (4), decrease, while $E_{d(a)}(r_{d(a)})$, $E_{gni(gpi)}(r_{d(a)})$, $N_{CDn(NDp)}(r_{d(a)})$, $N_{CDn(CDp)}^{EBT}(r_{d(a)})$, and $\frac{k_{Fn}^{-1}}{k_{sn}^{-1}}$, calculated using Equations (1, 1, 3, 21, 7), respectively, increase, affecting strongly all the physical properties, given in Sections 3-5

Donor		P	As	Te	Sb	Sn
r_d (nm) [4]	↗	0.110	0.118	0.132	0.136	0.140
$\varepsilon(r_d)$	↘	12.5	12.20	10.57	9.987	9.40
$a_{Bn}(r_d)$ in 10^{-7} cm	↘	9.07	8.86	7.67	7.25	6.87
$E_d(r_d)$ in meV	↗	6.35	6.67	8.88	9.95	11.23
$E_{gni}(r_d)$ in meV	↗	1424	1424.3	1426	1428	1429
$N_{CDn}(r_d)$ in 10^{16} cm^{-3}	↗	2.09	2.25	3.456	4.10	4.91
$N_{CDn}^{EBT}(r_d)$ in 10^{16} cm^{-3}	↗	2.09	2.24882	3.45636	4.0988	4.91274
$ RD $ in 10^{-4}		0	5.24	1.05	2.89	5.57
$\frac{k_{Fn}^{-1}}{k_{sn}^{-1}} < 1$ (Physical condition)		0.4012	0.4012	0.4012	0.4012	0.4012

Acceptor		Ga(Al)	Mg	In
r_a (nm) [4]	↗	0.126	0.140	0.144
$\varepsilon(r_a)$	↘	13.418	12.543	12.25
$a_{Bp}(r_a)$ in 10^{-7} cm	↘	2.098	1.96	1.95
$E_a(r_a)$ in meV	↗	25.60	29.30	29.51
$E_{gpi}(r_a)$ in meV	↗	1420	1423.8	1424
$N_{CDp}(r_a)$ in 10^{18} cm^{-3}	↗	1.692	2.072	2.090
$N_{CDp}^{EBT}(r_a)$ in 10^{18} cm^{-3}	↗	1.692	2.0713	2.0916
$ RD $ in 10^{-4}		0	3.45	7.61

$\frac{k_{\text{Fp}}^{-1}}{k_{\text{sp}}^{-1}} < 1$ (Physical condition)	0.3364	0.3364	0.3363
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Table 2 also indicates that, for increasing $r_{\text{d(a)}}$, both $\varepsilon(r_{\text{d(a)}})$ and $a_{\text{Bn(Bp)}}(r_{\text{d(a)}})$ decrease, while $E_{\text{d(a)}}(r_{\text{d(a)}})$, $E_{\text{gni(gpi)}}(r_{\text{d(a)}})$, $N_{\text{CDn(NDp)}}(r_{\text{d(a)}})$ and $N_{\text{CDn(CDp)}}^{\text{EBT}}(r_{\text{d(a)}})$ increase, affecting strongly all the physical properties, as those given in following Sections 3-5 .

3. Optical band gap

Here, $m_{\text{n(p)}}^*/m_0$ is chosen as: $m_{\text{n(p)}}^*/m_0 = m_{\text{r}}/m_0 = 0.060$, as given in Table 1 , and then, if denoting $N^* \equiv N - N_{\text{CDn(NDp)}}(r_{\text{d(a)}})$, the optical band gap (**OBG**) is found to be given by:

$$E_{\text{gn1(gp1)}}(N^*, r_{\text{d(a)}}, T) \equiv E_{\text{gn2(gp2)}}(N^*, r_{\text{d(a)}}, T) + E_{\text{Fn(Fp)}}(N^*, T), \quad (5)$$

where the reduced band gap is defined as:

$$E_{\text{gn2(gp2)}}(N^*, r_{\text{d(a)}}, T) \equiv E_{\text{gni(gpi)}}(r_{\text{d(a)}}) - \frac{4.9 \times 10^{-4} \times T^2 \text{ (eV)}}{T+327} - \Delta E_{\text{gn(gp)}}(N^*, r_{\text{d(a)}}). \quad (6)$$

Here, the intrinsic energy gap $E_{\text{gni(gpi)}}(r_{\text{d(a)}})$ is determined in Eq. (1), the Fermi energy $E_{\text{Fn(Fp)}}(N^*, T)$, in Eq. (A3), and the band gap narrowing $\Delta E_{\text{gn(gp)}}(N^*, r_{\text{d(a)}})$, in Equations (B3, B4), of the Appendix A and B, respectively. Then, as noted in the Appendix A and B, at $T=0\text{K}$, as $N^* = 0$, one has: $E_{\text{Fn(Fp)}}(N^*, T) \approx E_{\text{Fn0(Fp0)}}(N^*) = 0$, as given in Eq. (A4), and $\Delta E_{\text{gn(gp)}}(N^*, r_{\text{d(a)}}) = 0$, according to the MIT, as noted in Appendix A and B. Therefore, $E_{\text{gn1(gp1)}} = E_{\text{gn2(gp2)}} = E_{\text{gni(gpi)}}(r_{\text{d(a)}})$ at $T=0\text{K}$ and $N^* = 0$, according also to the MIT.

Finally, the numerical results of $E_{\text{gn1(gp1)}}(N^* > 0, r_{\text{d(a)}}, T)$ at $T=20\text{K}$, calculated using Eq. (5) and expressed as functions of N and $r_{\text{d(a)}}$, are reported in Table 3

Table 3. In degenerate d(a)- InP systems at $T=20\text{K}$, the numerical results of the OBG, evaluated using Eq. (5), suggesting that, for a given $r_{\text{d(a)}}$, the OBG increases with increasing N .

N (10^{18} cm^{-3})	4	8.5	15	50	80	100
$E_{\text{gn1}}(N^*, r_{\text{p}})$ in eV	1.506	1.580	1.671	2.045	2.302	2.457
$E_{\text{gn1}}(N^*, r_{\text{As}})$ in eV	1.505	1.579	1.669	2.041	2.298	2.452
$E_{\text{gn1}}(N^*, r_{\text{Te}})$ in eV	1.498	1.569	1.657	2.021	2.273	2.425
$E_{\text{gn1}}(N^*, r_{\text{Sb}})$ in eV	1.496	1.566	1.653	2.014	2.264	2.415
$E_{\text{gn1}}(N^*, r_{\text{Sn}})$ in eV	1.492	1.561	1.647	2.004	2.252	2.402
N (10^{18} cm^{-3})	6.5	11	15	26	60	170
$E_{\text{gp1}}(N^*, r_{\text{Ga(Al)}})$ in eV	1.506	1.573	1.626	1.753	2.072	2.847
$E_{\text{gp1}}(N^*, r_{\text{Mg}})$ in eV	1.500	1.566	1.619	1.745	2.061	2.830
$E_{\text{gp1}}(N^*, r_{\text{In}})$ in eV	1.499	1.566	1.618	1.745	2.060	2.829

Furthermore, in Table 3, we also showed that, in the n(p)-type degenerate InP and for a given photon energy $E \equiv \hbar\omega$, since the extinction coefficient, $\kappa_{n(p)}$, and other optical coefficients, as discussed in II, are expressed in terms of the function $(E - E_{gn1(gp1)})^{1/2}$. Therefore, if the values of $E_{gn1(gp1)}$ obtained in Table 3 increase (decrease), $(E - E_{gn})^{1/2}$ and other optical coefficients then decrease (increase), respectively.

4. Physical model and mathematical methods

4.1. Physical model

In the n(p)-type degenerate InP, if denoting the Fermi wave number by: $k_{Fn(Fp)}(N) \equiv (3\pi^2 N/g_{c(v)})^{1/3}$, the effective reduced Wigner-Seitz radius $r_{sn(sp)}$, characteristic of the interactions, is defined by

$$\gamma \times r_{sn(sp)}(N^*, r_{d(a)}, m_{n(p)}^*) \equiv \frac{k_{Fn(Fp)}^{-1}}{a_{Bn(Bp)}} < 1, \quad (6)$$

being proportional to $N^{*-1/3}$. Here, $\gamma = (4/9\pi)^{1/3}$, $k_{Fn(Fp)}^{-1}$ means the averaged distance between ionized donors (acceptors), and $a_{Bn(Bp)}(r_{d(a)})$ is determined in Eq. (4).

Then, the ratio of the inverse effective screening length $k_{sn(sp)}$ to Fermi wave number $k_{Fn(kp)}$ at 0 K is defined by

$$R_{sn(sp)}(N^*, r_{d(a)}) \equiv \frac{k_{sn(sp)}}{k_{Fn(Fp)}} = \frac{k_{Fn(Fp)}^{-1}}{k_{sn(sp)}^{-1}} = R_{snWS(spWS)} + [R_{snTF(spTF)} - R_{snWS(spWS)}]e^{-r_{sn(sp)}} < 1. \quad (7)$$

These ratios, $R_{snTF(spTF)}$ and $R_{snWS(spWS)}$, can be determined as follows.

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

$$R_{snTF}(N^*, r_{d(a)}) \equiv \frac{k_{snTF(spTF)}}{k_{Fn(Fp)}} = \frac{k_{Fn(Fp)}^{-1}}{k_{snTF(spTF)}^{-1}} = \sqrt{\frac{4\gamma r_{sn(sp)}}{\pi}} \ll 1, \quad (8)$$

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

$$R_{sn(sp)WS}(N^*, r_{d(a)}) \equiv \frac{k_{sn(sp)WS}}{k_{Fn}} = 0.5(1) \times \left(\frac{3}{2\pi} - \gamma^d \left[\frac{r_{sn(sp)}^2 \times E_{CE}(N^*, r_{d(a)})}{dr_{sn(sp)}} \right] \right), \quad (9)$$

where $E_{CE}(N^*, r_{d(a)})$ is the majority-carrier correlation energy (CE), being determined by Eq. (B2) of the Appendix B.

Furthermore, as given in II, in the degenerate case, the physical conditions are found to be given by :

$$\frac{k_{Fn(Fp)}^{-1}}{a_{Bn(Bp)}} < \frac{\eta_{n(p)}}{E_{Fno(Fpo)}} \equiv \frac{1}{A_{n(p)}} < \frac{k_{Fn(Fp)}^{-1}}{k_{sn(sp)}^{-1}} \equiv R_{sn(sp)} < 1, \quad A_{n(p)} \equiv \frac{E_{Fno(Fpo)}}{\eta_{n(p)}}, \quad (10)$$

being needed to determine the expression for electrical conductivity, as investigated in Section 5. Here, $R_{sn(sp)}$ is determined in Eq. (7).

Then, in degenerate d(a)-InP systems, 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 \vec{R}_j , randomly distributed throughout the Si crystal, is defined by

$$V(r) \equiv \sum_{j=1}^N v_j(r) + V_o, \quad (11)$$

where N is the total number of ionized donors(acceptors), V_o is a constant potential energy, and $v_j(r)$ is a screened Coulomb potential energy for each d(a)-Si system, defined as

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

where $k_{sn(sp)}$ is the inverse screening length determined in Eq. (7).

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

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

where Ω is the total InP -crystal volume.

Then, the effective auto-correlation function for potential fluctuations, $W_{n(p)}(v_{n(p)}, N^*, r_d) \equiv \langle V(r)V(r') \rangle$, was determined in II, as :

$$W_{n(p)}(v_{n(p)}, N^*, r_{d(a)}) \equiv \eta_{n(p)}^2 \times \exp\left(\frac{-\mathcal{H} \times R_{sn(sp)}(N^*, r_{d(a)})}{2\sqrt{|v_{n(p)}|}}\right), \quad \eta_{n(p)}(N^*, r_{d(a)}) \equiv \frac{\sqrt{2\pi N^*}}{\epsilon(r_{d(a)})} \times q^2 k_{sn(sp)}^{-1/2}, \quad v_{n(p)} \equiv \frac{-\mathbb{E}}{\mathbb{E}_{Fno(Fpo)}}. \quad (12)$$

Here, $\epsilon(r_{d(a)})$ is determined in Eq. (2), $R_{sn(sp)}(N^*, r_{d(a)})$ in Eq. (7), the empirical Heisenberg parameter $\mathcal{H} = 0.4721(1.585) = \mathcal{H}_{n(p)-InP}$ will be chosen such that the determination of the density of electrons localized in the conduction(valence)-band tails, given in Section 5, would be accurate, and finally $v_{n(p)} \equiv \frac{-\mathbb{E}}{\mathbb{E}_{Fno(Fpo)}}$, where \mathbb{E} is the total electron energy and $\mathbb{E}_{Fno(Fpo)}$ is the Fermi energy at 0 K, determined in Eq. (A4) of the Appendix A. In the following, we will calculate the ensemble average of the function: $(\mathbb{E} - V)^{a-\frac{1}{2}} \equiv \mathbb{E}_k^{a-\frac{1}{2}}$, for $a \geq 1$, $\mathbb{E}_k \equiv \frac{\hbar^2 \times k^2}{2 \times m_{n(p)}^*}$ being the kinetic energy of the electron (hole), and $V(r)$ determined in Eq. (11), by using the two following integration methods, as developed in II, which strongly depend on $W_{n(p)}(v_{n(p)}, N^*, r_{d(a)})$.

4.2. Mathematical methods and their application (Critical impurity density)

A. Kane integration method (KIM)

In heavily doped d(a)- InP systems, the effective Gaussian distribution probability is defined by

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

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

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

Then, by variable changes: $s = (\mathbb{E} - V)/\sqrt{W_{n(p)}}$ and $x = -\mathbb{E}/\sqrt{W_{n(p)}} \equiv A_{n(p)} \times v_{n(p)} \times \exp\left(\frac{\mathcal{H} \times R_{sn(sp)}}{4 \times \sqrt{|v_{n(p)}|}}\right)$,

and using an identity:

$$\int_0^\infty s^{a-\frac{1}{2}} \times \exp\left(-xs - \frac{s^2}{2}\right) ds \equiv \Gamma\left(a + \frac{1}{2}\right) \times \exp(x^2/4) \times D_{-a-\frac{1}{2}}(x),$$

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

$$\langle \mathbb{E}_k^{a-\frac{1}{2}} \rangle_{\text{KIM}} = \frac{\exp(-x^2/4) \times W_{n(p)}^{\frac{2a-1}{4}}}{\sqrt{2\pi}} \times \Gamma\left(a + \frac{1}{2}\right) \times D_{-a-\frac{1}{2}}(x) = \frac{\exp(-x^2/4) \times \eta_{n(p)}^{a-\frac{1}{2}}}{\sqrt{2\pi}} \times \exp\left(-\frac{\mathcal{H} \times R_{sn(sp)} \times (2a-1)}{8 \times \sqrt{|v_{n(p)}|}}\right) \times \Gamma\left(a + \frac{1}{2}\right) \times D_{-a-\frac{1}{2}}(x). \quad (13)$$

B. Feynman path-integral method (FPIM)

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

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

noting that as $a=1$, $(it)^{-\frac{3}{2}} \times \exp\left\{-\frac{(t\sqrt{W_{n(p)}})^2}{2\hbar^2}\right\}$ 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 $x = -\mathbb{E}/\sqrt{W_{n(p)}}$, and then using an identity:

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

one finally obtains: $\langle \mathbb{E}_k^{a-\frac{1}{2}} \rangle_{\text{FPIM}} \equiv \langle \mathbb{E}_k^{a-\frac{1}{2}} \rangle_{\text{KIM}}$, $\langle \mathbb{E}_k^{a-\frac{1}{2}} \rangle_{\text{KIM}}$ being determined in Eq. (13).

In the following, with use of asymptotic forms for $D_{-a-\frac{1}{2}}(x)$, those given for $\langle (\mathbb{E} - V)^{a-\frac{1}{2}} \rangle_{\text{KIM}}$ will be obtained in the two cases: $\mathbb{E} \geq 0$ and $\mathbb{E} \leq 0$.

(i) $\mathbb{E} \geq 0$ -case

As $\mathbb{E} \rightarrow +\infty$, one has: $v_n \rightarrow -\infty$ and $x \rightarrow -\infty$. In this case, one gets:

$$D_{-a-\frac{1}{2}}(x \rightarrow -\infty) \approx \frac{\sqrt{2\pi}}{\Gamma(a+\frac{1}{2})} \times e^{\frac{x^2}{4}} \times (-x)^{a-\frac{1}{2}}.$$

Therefore, Eq. (13) becomes: $\langle \mathbb{E}_k^{a-\frac{1}{2}} \rangle_{\text{KIM}} \approx \mathbb{E}^{a-\frac{1}{2}}$. Further, as $\mathbb{E} \rightarrow +0$, one has: $v_{n(p)} \rightarrow -0$ and $x \rightarrow -\infty$. So, one gets :

$$D_{-a-\frac{1}{2}}(x \rightarrow -\infty) \simeq \beta(a) \times \exp\left(\left(\sqrt{a} + \frac{1}{3}\right)x - \frac{x^2}{16a} + \frac{x^3}{24\sqrt{a}}\right) \rightarrow 0, \quad \beta(a) = \frac{\sqrt{\pi}}{2^{\frac{2a+1}{4}} \Gamma(\frac{a}{2} + \frac{3}{4})}.$$

Thus, as $\mathbb{E} \rightarrow +0$, from Eq. (13), one gets: $\langle \mathbb{E}_k^{a-\frac{1}{2}} \rangle_{\text{KIM}} \rightarrow 0$.

In summary, for $\mathbb{E} \geq 0$, the expression of $\langle \mathbb{E}_k^{a-\frac{1}{2}} \rangle_{\text{KIM}}$ can be approximated by:

$$\langle \mathbb{E}_k^{a-\frac{1}{2}} \rangle_{\text{KIM}} \cong \mathbb{E}^{a-\frac{1}{2}}, \quad \mathbb{E}_k \equiv \frac{\hbar^2 \times k^2}{2 \times m^*}. \quad (14)$$

(ii) $\mathbb{E} \leq 0$ – case.

As $\mathbb{E} \rightarrow -0$, from Eq. (13), one has: $v_{n(p)} \rightarrow +0$ and $x \rightarrow +\infty$. Thus, one first obtains, for any $a \geq 1$,

$$D_{-a-\frac{1}{2}}(x \rightarrow \infty) \simeq \beta(a) \times \exp \left[-(\sqrt{a} + \frac{1}{3})x - \frac{x^2}{16a} - \frac{x^3}{24\sqrt{a}} \right] \rightarrow 0, \quad \beta(a) = \frac{\sqrt{\pi}}{2^{\frac{2a+1}{4}} \Gamma(\frac{a+3}{4})}, \text{ noting that}$$

$$\beta(1) = \frac{\sqrt{\pi}}{2^{\frac{3}{4}} \Gamma(5/4)} \text{ and } \beta(5/2) = \frac{\sqrt{\pi}}{2^{3/2}}.$$

Then, 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. (13) yields

$$H_{n(p)}(v_{n(p)} \rightarrow +0, r_{d(a)}, a) = \frac{\langle \mathbb{E}_k^{a-\frac{1}{2}} \rangle_{\text{KIM}}}{f(a)} = \exp \left[-\frac{\mathcal{H} \times R_{\text{sn(sp)}} \times (2a-1)}{8 \times \sqrt{|v_{n(p)}|}} - \left(\sqrt{a} + \frac{1}{3} \right) x - \frac{(\frac{1}{4} + \frac{1}{16a})x^2 - \frac{x^3}{24\sqrt{a}}}{16a^2} \right] \rightarrow 0. \quad (15)$$

Further, as $\mathbb{E} \rightarrow -\infty$, one has: $v_{n(p)} \rightarrow +\infty$ and $x \rightarrow \infty$. Thus, one gets:

$$D_{-a-\frac{1}{2}}(x \rightarrow \infty) \approx x^{-a-\frac{1}{2}} \times e^{-\frac{x^2}{4}} \rightarrow 0. \text{ Therefore, Eq. (13) yields}$$

$$K_{n(p)}(v_{n(p)} \rightarrow +\infty, r_{d(a)}, a) \equiv \frac{\langle \mathbb{E}_k^{a-\frac{1}{2}} \rangle_{\text{KIM}}}{f(a)} \simeq \frac{1}{\beta(a)} \times \exp \left(-\frac{(A_{n(p)} \times v_{n(p)})^2}{2} \right) \times (A_{n(p)} \times v_{n(p)})^{-a-\frac{1}{2}} \rightarrow 0. \quad (16)$$

It should be noted that, as $\mathbb{E} \leq 0$, the ratios (15) and (16) can be taken in an approximate form as:

$$F_{n(p)}(v_{n(p)}, r_{d(a)}, a) = K_{n(p)}(v_{n(p)}, r_{d(a)}, a) + [H_{n(p)}(v_{n(p)}, r_{d(a)}, a) - K_{n(p)}(v_{n(p)}, r_{d(a)}, a)] \times \exp [-c_1 \times (A_{n(p)} v_{n(p)})^{c_2}], \quad (17)$$

such that: $F_{n(p)}(v_{n(p)}, r_{d(a)}, a) \rightarrow H_{n(p)}(v_{n(p)}, r_{d(a)}, a)$ for $0 \leq v_n \leq 16$, and $F_{n(p)}(v_{n(p)}, r_{d(a)}, a) \rightarrow K_{n(p)}(v_{n(p)}, r_{d(a)}, a)$ for $v_{n(p)} \geq 16$. 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), $N_{\text{CDn(CDp)}}^{\text{EBT}}(N, r_{d(a)})$, in the following.

C. Critical impurity density in the MIT

In degenerate d(a)- InP systems at $T=0$ K, in which $m_{n(p)}^*/m_0 = m_{n(p)}/m_0 = 0.073(0.339)$, as given in Table 1, using Eq. (13), for $a=1$, the density of states $\mathcal{D}(\mathbb{E})$ is defined by:

$$\langle \mathcal{D}(\mathbb{E}_k) \rangle_{\text{KIM}} \equiv \frac{g_c(v)}{2\pi^2} \left(\frac{2m_{n(p)}}{\hbar^2} \right)^{\frac{3}{2}} \times \langle \mathbb{E}_k^{\frac{1}{2}} \rangle_{\text{KIM}} = \frac{g_c(v)}{2\pi^2} \left(\frac{2m_{n(p)}}{\hbar^2} \right)^{\frac{3}{2}} \times \frac{\exp \left(-\frac{x^2}{4} \right) \times W_n^{\frac{1}{4}}}{\sqrt{2\pi}} \times \Gamma\left(\frac{3}{2}\right) \times D_{-\frac{3}{2}}(x) = \mathcal{D}(\mathbb{E}), \quad (18)$$

where x is defined in Eq. (13), as: $x = -\mathbb{E}/\sqrt{W_{n(p)}} \equiv A_{n(p)} \times v_{n(p)} \times \exp \left(\frac{\mathcal{H} \times R_{\text{sn(sp)}}}{4 \times \sqrt{|v_{n(p)}|}} \right)$.

Here, \mathbb{E}_{Fno} is determined in Eq. (A4) of the Appendix A, with $m_{n(p)}^*/m_0 = m_{n(p)}/m_0$ and $\mathcal{H} = 0.4721(1.585)$, being chosen such that the following determination of $N_{\text{CDn(CDp)}}^{\text{EBT}}(N, r_{d(a)})$ would be accurate.

Then, going back to the functions: H_n , K_n and F_n , given respectively in Equations (15-17), in which the

factor $\frac{\langle \mathbb{E}_k^2 \rangle_{\text{KIM}}}{f(a=1)}$ is now replaced by:

$$\frac{\langle \mathbb{E}_k^2 \rangle_{\text{KIM}}}{f(a=1)} = \frac{\mathcal{D}(\mathbb{E} \leq 0)}{\mathcal{D}_0} = F_{n(p)}(v_{n(p)}, r_{d(a)}, a = 1), \quad \mathcal{D}_0 = \frac{g_{c(v)} \times (m_{n(p)} \times m_o)^{3/2} \times \sqrt{\eta_{n(p)}}}{2\pi^2 \hbar^3} \times \beta(a = 1), \quad \beta(a = 1) = \frac{\sqrt{\pi}}{2^4 \times \Gamma(5/4)}. \quad (19)$$

Therefore, the densities of electrons (holes) localized in exponential conduction (valence)-band tails, $N_{\text{CDn(CDp)}}^{\text{EBT}}(N, r_{d(a)})$, can be defined by

$$N_{\text{CDn(CDp)}}^{\text{EBT}}(N, r_{d(a)}) = \int_{-\infty}^0 \mathcal{D}(\mathbb{E} \leq 0) d\mathbb{E},$$

where $\mathcal{D}(\mathbb{E} \leq 0)$ is determined in Eq. (19). Then, by a variable change: $v_{n(p)} \equiv \frac{-\mathbb{E}}{\mathbb{E}_{\text{Fno(Fpo)}}$, one obtains:

$$N_{\text{CDn(CDp)}}^{\text{EBT}}(N, r_{d(a)}) = \frac{g_{c(v)} \times (m_{n(p)})^{3/2} \sqrt{\eta_{n(p)}} \times \mathbb{E}_{\text{Fno(Fpo)}}}{2\pi^2 \hbar^3} \times \left\{ \int_0^{16} \beta(a = 1) \times F_{n(p)}(v_{n(p)}, r_{d(a)}, a = 1) dv_{n(p)} + I_{n(p)} \right\}, \quad (20)$$

where

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

$$\text{Here, } \beta(a = 1) = \frac{\sqrt{\pi}}{2^4 \times \Gamma(5/4)}.$$

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

$$I_{n(p)} = \frac{1}{2^{5/4} A_{n(p)}} \times \int_{y_{n(p)}}^{\infty} t^{b-1} e^{-t} dt \equiv \frac{\Gamma(b, y_{n(p)})}{2^{5/4} \times A_{n(p)}},$$

where $b = -1/4$, $y_{n(p)} = [16 A_{n(p)} / \sqrt{2}]^2$, and $\Gamma(b, y_{n(p)})$ is the incomplete Gamma function, defined by:

$$\Gamma(b, y_{n(p)}) = y_{n(p)}^{b-1} \times e^{-y_{n(p)}} \left[1 + \sum_{j=1}^{16} \frac{(b-1)(b-2)\dots(b-j)}{y_{n(p)}^j} \right].$$

Finally, Eq. (20) now yields:

$$N_{\text{CDn(CDp)}}^{\text{EBT}}(N, r_{d(a)}) = \frac{g_{c(v)} \times (m_{n(p)})^{3/2} \sqrt{\eta_{n(p)}} \times \mathbb{E}_{\text{Fno(Fpo)}}}{2\pi^2 \hbar^3} \times \left\{ \int_0^{16} \beta(a = 1) \times F_{n(p)}(v_{n(p)}, r_{d(a)}, a = 1) dv_{n(p)} + \frac{\Gamma(b, y_{n(p)})}{2^{5/4} \times A_{n(p)}} \right\}, \quad \text{calculated for } N = N_{\text{CDn(NDp)}}(r_{d(a)}), \quad (21)$$

being the density of electrons localized in the exponential conduction-band tails (EBT).

The numerical results of $N_{\text{CDn(CDp)}}^{\text{EBT}}[N = N_{\text{CDn(NDp)}}(r_{d(a)})] = N_{\text{CDn(CDp)}}^{\text{EBT}}(r_{d(a)})$, evaluated using Eq. (21), are given in Table 2, confirming thus those of $N_{\text{CDn(NDp)}}(r_{d(a)})$, calculated using Eq. (3), with a precision of the order of $5.57(7.61) \times 10^{-4}$, respectively. In other word, $N_{\text{CDn(NDp)}}(r_{d(a)})$, determined in Eq. (3), can be explained by $N_{\text{CDn(CDp)}}^{\text{EBT}}(r_{d(a)})$, determined in Eq. (21).

5. Fermi-Dirac distribution function at low temperatures, and its applications

5.1. Fermi-Dirac distribution function (FDDF) at low temperatures

The Fermi-Dirac distribution function (FDDF) is given by

$$f(\mathbb{E}) \equiv (1 + e^\gamma)^{-1}, \quad \gamma \equiv (\mathbb{E} - \mathbb{E}_{\text{Fn}(\text{Fp})})/(k_B T),$$

where $\mathbb{E}_{\text{Fn}(\text{Fp})}(N, T)$ is the Fermi energy determined in Eq. (A3) of the Appendix A.

So, the average of \mathbb{E}^p , calculated using the FDDF-method, as developed in II, can be defined as:

$$\langle \mathbb{E}^p \rangle_{\text{FDDF}} \equiv G_p(\mathbb{E}_{\text{Fn}}) \times \mathbb{E}_{\text{Fn}}^p \equiv \int_{-\infty}^{\infty} \mathbb{E}^p \times \left(-\frac{\partial f}{\partial \mathbb{E}} \right) d\mathbb{E}, \quad -\frac{\partial f}{\partial \mathbb{E}} = \frac{1}{k_B T} \times \frac{e^\gamma}{(1+e^\gamma)^2}. \quad (22)$$

Further, one notes that, at 0 K, $-\frac{\partial f}{\partial \mathbb{E}} = \delta(\mathbb{E} - \mathbb{E}_{\text{Fn}(\text{Fpo})})$, $\delta(\mathbb{E} - \mathbb{E}_{\text{Fn}(\text{Fpo})})$ being the Dirac delta (δ)-function and $\mathbb{E}_{\text{Fn}(\text{Fpo})}$ is the Fermi energy at $T=0$ K defined in Eq. (A4) of the Appendix A. Therefore, $G_p(\mathbb{E}_{\text{Fn}(\text{Fpo})}) = 1$.

Then, at low T, by a variable change $\gamma \equiv (\mathbb{E} - \mathbb{E}_{\text{Fn}(\text{Fp})})/(k_B T)$, Eq. (22) yields:

$$G_p(\mathbb{E}_{\text{Fn}(\text{Fp})}) \equiv 1 + \mathbb{E}_{\text{Fn}(\text{Fp})}^{-p} \times \int_{-\infty}^{\infty} \frac{e^\gamma}{(1+e^\gamma)^2} \times (k_B T \gamma + \mathbb{E}_{\text{Fn}(\text{Fp})})^p d\gamma = 1 + \sum_{\mu=1,2,\dots}^p C_p^\beta \times (k_B T)^\beta \times \mathbb{E}_{\text{Fn}(\text{Fp})}^{-\beta} \times I_\beta,$$

where $C_p^\beta \equiv p(p-1)\dots(p-\beta+1)/\beta!$ and the integral I_β is given by:

$$I_\beta = \int_{-\infty}^{\infty} \frac{\gamma^\beta \times e^\gamma}{(1+e^\gamma)^2} d\gamma = \int_{-\infty}^{\infty} \frac{\gamma^\beta}{(e^{\gamma/2} + e^{-\gamma/2})^2} d\gamma, \text{ vanishing for odd values of } \beta. \text{ Then, for even values of } \beta = 2n,$$

with $n=1, 2, \dots$, one obtains:

$$I_{2n} = 2 \int_0^{\infty} \frac{\gamma^{2n} \times e^\gamma}{(1+e^\gamma)^2} d\gamma. \quad (23)$$

Now, using an identity $(1 + e^\gamma)^{-2} \equiv \sum_{s=1}^{\infty} (-1)^{s+1} s \times e^{\gamma(s-1)}$, a variable change: $s\gamma = -t$, the Gamma function: $\int_0^{\infty} t^{2n} e^{-t} dt \equiv \Gamma(2n+1) = (2n)!$, and also the definition of the Riemann's zeta function: $\zeta(2n) \equiv 2^{2n-1} \pi^{2n} |B_{2n}|/(2n)!$, B_{2n} being the Bernoulli numbers, one finally gets: $I_{2n} = (2^{2n} - 2) \times \pi^{2n} \times |B_{2n}|$. So, from Eq. (22), we get in the degenerate case the following ratio:

$$G_p(\mathbb{E}_{\text{Fn}(\text{Fp})}) \equiv \frac{\langle \mathbb{E}^p \rangle_{\text{FDDF}}}{\mathbb{E}_{\text{Fn}(\text{Fp})}^p} = 1 + \sum_{n=1}^p \frac{p(p-1)\dots(p-2n+1)}{(2n)!} \times (2^{2n} - 2) \times |B_{2n}| \times y^{2n} \equiv G_p(y), \quad y = \frac{\pi k_B T}{\mathbb{E}_{\text{Fn}(\text{Fp})}}. \quad (24)$$

Then, some usual results of $G_p(y)$ are given in Table 4.

Table 4. Expressions for $G_{p \geq 1}(y \equiv \frac{\pi}{\xi_{n(p)}})$, as given in II, due to the Fermi-Dirac distribution function FDDF, noting

that $G_{p=1}(y \equiv \frac{\pi k_B T}{\mathbb{E}_{\text{Fn}(\text{Fp})}} = \frac{\pi}{\xi_{n(p)}}) = 1$, used to determine the electrical-and-thermoelectric coefficients in Section 5

$G_{3/2}(y)$	$G_2(y)$	$G_{5/2}(y)$	$G_3(y)$	$G_{7/2}(y)$	$G_4(y)$	$G_{9/2}(y)$
$\left(1 + \frac{y^2}{8} + \frac{7y^4}{640}\right)$	$\left(1 + \frac{y^2}{3}\right)$	$\left(1 + \frac{5y^2}{8} - \frac{7y^4}{384}\right)$	$(1 + y^2)$	$\left(1 + \frac{35y^2}{24} + \frac{49y^4}{384}\right)$	$\left(1 + 2y^2 + \frac{7y^4}{15}\right)$	$\left(1 + \frac{21y^2}{8} + \frac{147y^4}{128}\right)$

These functions $G_p(y)$ will be applied to determine the majority-carrier transport coefficients given in the $n(p)$ -type degenerate InP, as follows.

5. 2. Its applications (Electrical-and-thermoelectric properties)

Here, $m_{n(p)}^*/m_o$ is chosen as: $m_{n(p)}^*/m_o = m_{Cn(Cp)}/m_o = 0.077(0.50)$, as given in Table 1, and all the majority-carrier transport coefficients are expressed as functions of the effective donor (acceptor)-density as: $N^* \equiv N - N_{CDn(NDp)}(r_{d(a)})$, where the values of critical d(a)-densities $N_{CDn(NDp)}(r_{d(a)})$ are given in Table 2. As given in II, if denoting, for majority electrons (holes), the electrical conductivity by $\sigma(N^*, r_{d(a)}, T)$, expressed in $\text{ohm}^{-1} \times \text{cm}^{-1}$, the thermal conductivity by $\kappa(N^*, r_{d(a)}, T)$, expressed in $\frac{W}{\text{cm} \times K}$, and Lorenz number by $L = \frac{\pi^2}{3} \times \left(\frac{k_B}{q}\right)^2 = 2.4429637 \left(\frac{W \times \text{ohm}}{K^2}\right)$, then the well-known Wiedemann-Frank law states that the ratio, $\frac{\kappa}{\sigma}$, is proportional to the temperature $T(K)$, as:

$$\frac{\kappa(N^*, r_{d(a)}, T)}{\sigma(N^*, r_{d(a)}, T)} = L \times T. \quad (25a)$$

Then, it is interesting to define a constant $C_\kappa(N^*, r_{d(a)}) \equiv \frac{\kappa(N^*, r_{d(a)}, T=3K)}{L}$ in order to show that, for given N^* and $r_{d(a)}$, $\kappa_{App.}(N^*, r_{d(a)}, T)$ is found to be proportional to T , as:

$$\kappa_{App.}(N^*, r_{d(a)}, T) \simeq C_\kappa(N^*, r_{d(a)}) \times T, \quad \left| RD_{\kappa, \kappa_{App.}} \right|_T \equiv \left| 1 - \frac{\kappa_{App.}(N^*, r_{d(a)}, T)}{\kappa(N^*, r_{d(a)}, T)} \right|, \quad (25b)$$

where $\left| RD_{\kappa, \kappa_{App.}} \right|_T$ is the relative deviations in absolute values between $\kappa(N^*, r_{d(a)}, T)$ and $\kappa_{App.}(N^*, r_{d(a)}, T)$, as a function of T .

Thus, if σ is known, κ and other majority-carrier transport coefficients are also determined, since those are related to σ . We now determine the general form of σ in the following.

First, it is expressed in terms of the kinetic energy of the electron (hole), $\mathbb{E}_k \equiv \frac{\hbar^2 \times k^2}{2 \times m_{Cn(Cp)}}$, or the wave number k , as:

$$\sigma(k) \equiv C \times \frac{q^2 \times k}{\pi \times \hbar} \times \frac{k}{k_{sn(sp)}} \times [k \times a_{Bn(Bp)}(r_{d(a)})] \times \left(\frac{\mathbb{E}_k}{\eta_{n(p)}(N, r_{d(a)})} \right)^{1/2}, \quad C = (0.89645)^2, \quad (26)$$

which is thus proportional to \mathbb{E}_k^2 . Further, $k_{sn(sp)}$, $a_{Bn(Bp)}$, and $\eta_{n(p)}$ are defined and determined in Equations (7, 4, 12), respectively.

Then, from Eq. (14), for $\mathbb{E} \geq 0$, we get: $\langle \mathbb{E}_k^2 \rangle_{KIM} \cong \mathbb{E}^2$, and from Eq. (22) we obtain: $\langle \mathbb{E}^2 \rangle_{FDDF} \equiv G_2(y = \frac{\pi k_B T}{\mathbb{E}_{Fn(Fp)}}) \times \mathbb{E}_{Fn(Fp)}^2$, where $\mathbb{E}_{Fn(Fp)}$ is the Fermi energy, determined in Eq. (A3) of the Appendix A, and

$G_2(y) = \left(1 + \frac{y^2}{3}\right) \equiv G_2(N^*, T)$ is given in Table 4. Therefore, Eq. (26) becomes as:

$$\sigma(N^*, r_{d(a)}, T) \equiv \left[C \times \frac{q^2 \times k_{Fn(Fp)}}{\pi \times \hbar} \times \frac{k_{Fn(Fp)}}{k_{sn(sp)}} \times [k_{Fn(Fp)} \times a_{Bn(Bp)}(r_{d(a)})] \times \left(\frac{\mathbb{E}_{Fno(Fpo)}(N^*, T=0)}{\eta_{n(p)}(N, r_{d(a)})} \right)^{1/2} \right] \times [G_2(N^*, T) \times \left(\frac{\mathbb{E}_{Fn(Fp)}(N^*, T)}{\mathbb{E}_{Fno(Fpo)}(N^*, T=0)} \right)^2], \quad (27)$$

which also determine the resistivity as: $\rho(N^*, r_{d(a)}, T) \equiv 1/\sigma(N^*, r_{d(a)}, T)$, noting that $N^* \equiv N - N_{CDn(NDp)}(r_{d(a)})$, and $C \times \frac{q^2}{\pi \times \hbar} = 6.226527 \times 10^{-5} \text{ ohm}^{-1}$. Further, the Fermi energies $E_{Fn(Fp)}$ and $E_{Fno(Fpo)}$ are determined respectively in Equations (A3, A4) of the Appendix A.

In Eq. (27), one notes that at $T = 0 \text{ K}$, as noted in Eq. (22), $\sigma(N^*, r_{d(a)}, T = 0 \text{ K})$ is proportional to $E_{Fno(Fpo)}^2$, or to $(N^*)^{4/3}$. Thus, $\sigma(N^* = 0, r_{d(a)}, T = 0 \text{ K}) = 0$ at $N^* = 0$, at which the metal-insulator transition (MIT) occurs.

A. Electrical properties

As given in II, the relaxation time τ is related with σ by:

$$\tau(N^*, r_{d(a)}, T) \equiv \sigma(N^*, r_{d(a)}, T) \times \frac{m_{Cn(Cp)}}{q^2 \times N^*} . \text{ Therefore, the mobility } \mu \text{ is given by:}$$

$$\mu(N^*, r_{d(a)}, T) \equiv \frac{q \times \tau(N^*, r_{d(a)}, T)}{m_{Cn(Cp)}} = \frac{\sigma(N^*, r_{d(a)}, T)}{q \times N^*} . \quad (28)$$

In Eq. (28), at $T = 0 \text{ K}$, $\mu(N^*, r_{d(a)}, T = 0 \text{ K})$ is thus proportional to $(N^*)^{1/3}$, since $\sigma(N^*, r_{d(a)}, T = 0 \text{ K})$ is proportional to $(N^*)^{4/3}$. Thus , $\mu(N^* = 0, r_{d(a)}, T = 0 \text{ K}) = 0$ at $N^* = 0$, at which the metal-insulator transition (MIT) occurs.

Then, since τ and σ are both proportional to E^2 , as given above, the Hall factor can thus be determined by:

$$r_H(N^*, T) \equiv \frac{\langle \tau^2 \rangle_{FDDF}}{[\langle \tau \rangle_{FDDF}]^2} = \frac{G_4(y)}{[G_2(y)]^2}, \text{ and therefore, the Hall mobility yields:}$$

$$\mu_H(N^*, r_{d(a)}, T) \equiv \mu(N^*, r_{d(a)}, T) \times r_H(N^*, T), \quad (29)$$

noting that, at $T = 0 \text{ K}$, since $r_H(N^*, T = 0 \text{ K}) = 1$, one gets:

$$\mu_H(N^* = 0, r_{d(a)}, T = 0 \text{ K}) \equiv \mu(N^* = 0, r_{d(a)}, T = 0 \text{ K}) = 0 \text{ at } N^* = 0, \text{ at which the metal-insulator transition (MIT) occurs.}$$

Now, in the degenerate d(a)-InP systems, at $T = 4.2 \text{ K}$ and $T = 77 \text{ K}$, the numerical results of σ , μ , μ_H , and the diffusion coefficient D , calculated respectively by using Equations (27, 28, 29, A8 of the Appendix A), and reported in following Tables 5 and 6.

Table 5. Here, one notes that: (i) for given N and T , the functions: $\sigma(r_d)$, $\mu(r_d)$, $\mu_H(r_d)$ and $D(r_d)$, calculated using respective Equations (27, 28, 29, A8 of the Appendix A), decrease with increasing r_d , and (ii) for given r_d and T , the functions: $\sigma(N^*)$ and $D(N^*)$ increase, while the functions: $\mu(N^*)$ and $\mu_H(N^*)$ decrease, with increasing N .

Donor	P	As	Te	Sb	Sn
In the following, our numerical results of (σ, μ, μ_H, D) at 4.2K, expressed respectively in $\left(\frac{10^5}{\text{ohm} \times \text{cm}}, \frac{10^3 \times \text{cm}^2}{\text{V} \times \text{s}}, \frac{10^3 \times \text{cm}^2}{\text{V} \times \text{s}}, \frac{10^3 \times \text{cm}^2}{\text{s}} \right)$					
$N(10^{19} \text{ cm}^{-3})$					
3	0.446, 9.29, 9.29, 3.25	0.427, 8.89, 8.89, 3.11	0.332, 6.91, 6.91, 2.4	0.300, 6.25, 6.25, 2.2	0.270, 5.63, 5.63, 2.0
10	1.37, 8.55, 8.55, 6.68	1.31, 8.18, 8.18, 6.39	1.01, 6.32, 6.32, 4.94	0.914, 5.70, 5.70, 4.46	0.820, 5.12, 5.12, 4.0
40	5.06, 7.90, 7.90, 15.6	4.84, 7.55, 7.55, 14.88	3.72, 5.81, 5.81, 11.4	3.35, 5.23, 5.23, 10.3	3.002, 4.68, 4.68, 9.22
70	8.61, 7.68, 7.68, 21.9	8.23, 7.34, 7.34, 20.1	6.32, 5.63, 5.63, 16.1	5.69, 5.07, 5.07, 14.5	5.09, 4.54, 4.54, 13.0
100	12.08, 7.54, 7.54, 27.4	11.5, 7.21, 7.21, 26.1	8.86, 5.53, 5.53, 20.0	7.98, 4.98, 4.98, 18.1	7.13, 4.45, 4.45, 16.1

In the following, our numerical results of (σ, μ, μ_H, D) at **77K**, expressed respectively in $\left(\frac{10^5}{\text{ohm}\times\text{cm}}, \frac{10^3\times\text{cm}^2}{\text{V}\times\text{s}}, \frac{10^3\times\text{cm}^2}{\text{V}\times\text{s}}, \frac{10^3\times\text{cm}^2}{\text{s}}\right)$
 $N(10^{19}\text{ cm}^{-3})$

3	0.446, 9.29, 9.31, 3.2	0.427, 8.90, 8.92, 3.1	0.332, 6.91, 6.92, 2.4	0.300, 6.26, 6.27, 2.2	0.270, 5.63, 5.64, 1.97
10	1.37, 8.55, 8.56, 6.68	1.31, 8.18, 8.19, 6.40	1.01, 6.32, 6.32, 4.94	0.914, 5.71, 5.71, 4.46	0.820, 5.12, 5.12, 4.0
40	5.06, 7.90, 7.90, 15.5	4.84, 7.55, 7.56, 14.9	3.72, 5.81, 5.81, 11.4	3.35, 5.23, 5.23, 10.3	3.00, 4.68, 4.68, 9.22
70	8.61, 7.68, 7.68, 21.9	8.23, 7.34, 7.34, 21.0	6.32, 5.63, 5.63, 16.1	5.69, 5.07, 5.07, 14.5	5.09, 4.54, 4.54, 13.0
100	12.1, 7.54, 7.54, 27.4	11.5, 7.21, 7.21, 26.1	8.86, 5.53, 5.53, 20.0	7.98, 4.98, 4.98, 18.1	7.13, 4.45, 4.45, 16.1

Table 6. Here, one notes that: (i) for given N and T , the functions: $\sigma(r_a)$, $\mu(r_a)$, $\mu_H(r_a)$ and $D(r_a)$, calculated using respective Equations (27, 28, 29, A8 of the Appendix A), decrease with increasing r_a , and (ii) for given r_a and T , the functions: $\sigma(N^*)$ and $D(N^*)$ increase, while the functions: $\mu(N^*)$ and $\mu_H(N^*)$ decrease, with increasing N .

Acceptor	Ga(Al)	Mg	In
In the following, our numerical results of (σ, μ, μ_H, D) at 4.2K , expressed respectively in $\left(\frac{10^4}{\text{ohm}\times\text{cm}}, \frac{10^2\times\text{cm}^2}{\text{V}\times\text{s}}, \frac{10^2\times\text{cm}^2}{\text{V}\times\text{s}}, \frac{10^2\times\text{cm}^2}{\text{s}}\right)$ $N(10^{19}\text{ cm}^{-3})$			
3	0.185, 4.07, 4.07, 0.18	0.168, 3.75, 3.75, 0.17	0.167, 3.73, 3.73, 0.17
10	0.49, 3.11, 3.12, 0.32	0.445, 2.83, 2.83, 0.29	0.443, 2.82, 2.82, 0.29
40	1.58, 2.48, 2.48, 0.65	1.42, 2.23, 2.23, 0.59	1.41, 2.22, 2.22, 0.58
70	2.57, 2.30, 2.30, 0.88	2.30, 2.06, 2.06, 0.79	2.29, 2.05, 2.05, 0.78
100	3.52, 2.20, 2.20, 1.07	3.15, 1.97, 1.97, 0.96	3.13, 1.96, 1.96, 0.95
In the following, our numerical results of (σ, μ, μ_H, D) at 77K , expressed respectively in $\left(\frac{10^4}{\text{ohm}\times\text{cm}}, \frac{10^2\times\text{cm}^2}{\text{V}\times\text{s}}, \frac{10^2\times\text{cm}^2}{\text{V}\times\text{s}}, \frac{10^2\times\text{cm}^2}{\text{s}}\right)$ $N(10^{19}\text{ cm}^{-3})$			
3	0.190, 4.20, 4.70, 0.19	0.173, 3.87, 4.33, 0.18	0.172, 3.85, 4.532, 0.17
10	0.49, 3.14, 3.21, 0.33	0.447, 2.85, 2.92, 0.29	0.445, 2.84, 2.91, 0.29
40	1.58, 2.48, 2.49, 0.65	1.42, 2.23, 2.24, 0.59	1.14, 2.22, 2.23, 0.58
70	2.57, 2.30, 2.30, 0.88	2.31, 2.06, 2.07, 0.79	2.29, 2.05, 2.05, 0.78
100	3.52, 2.20, 2.21, 1.07	3.15, 1.97, 1.97, 0.96	3.13, 1.96, 1.96, 0.95

B. Thermoelectric properties

First off all, from Eq. (27), obtained for $\sigma(N^*, r_{d(a)}, T)$, the well-known Mott definition for the thermoelectric

power or for the Seebeck coefficient, S_b , is given in the n(p)-type degenerate InP, as:

$$S_b(N^*, T) \equiv (\mp) \frac{\pi^2}{3} \times \frac{k_B}{q} \times k_B T \times \left. \frac{\partial \ln \sigma(E)}{\partial E} \right|_{E=E_{Fn}(Fp)}.$$

Then, using Eq. (27), for $\xi_{n(p)} \equiv \frac{E_{Fn}(Fp)(N^*, T)}{k_B T} \gtrsim 1$, one gets:

$$S_b(N^*, T) \equiv (\mp) \frac{\pi^2}{3} \times \frac{k_B}{q} \times \frac{2}{\frac{\pi^2}{3} \xi_{n(p)}} \times F_{Sb}(N^*, T), \quad F_{Sb}(N^*, T) \equiv \left[1 - \frac{y^2}{3 \times G_2(y = \frac{\pi k_B T}{E_{Fn}(Fp)(N^*, T)})} \right], \quad (30)$$

noting that the effective donor (acceptor) density, $N^* \equiv N - N_{CDn}(r_{d(a)})$, is a function of $r_{d(a)}$.

Therefore, the Thomson coefficient, T_s , is given by:

$$T_s(N^*, T) \equiv T \times \frac{dSb(N^*, T)}{dT}, \quad (31)$$

and then, the Peltier coefficient, P_t , is defined as:

$$P_t(N^*, T) \equiv T \times Sb(N^*, T). \quad (32)$$

Finally, from Equations (25a, 30), one can define the figure of merit, ZT , by:

$$ZT(N^*, T) \equiv \frac{[Sb(N^*, T)]^2 \times \sigma(N^*, r_{d(a)}, T) \times T}{\kappa(N^*, r_{d(a)}, T)} = \frac{[Sb(N^*, T)]^2}{L} = (ZT)_{Mott} \times [2 \times F_{Sb}(N^*, T)]^2, \quad (ZT)_{Mott} = \frac{\pi^2}{3 \times \xi_{n(p)}^2}, \quad (33)$$

where $(ZT)_{Mott}$ is a well-known Mott result, $L = \frac{\pi^2}{3} \times \left(\frac{k_B}{q}\right)^2 = 2.4429637 \times 10^{-8} \left(\frac{W \times ohm}{K^2}\right)$ is the Lorenz number, noting that, in the n(p)-type degenerate InP $\left[\xi_{n(p)} \equiv \frac{E_{Fn(Fp)}(N^*, T)}{k_B T} \geq 1\right]$, this value of L is exact, and confirmed in the following.

It should be noted that Kim et al. [11] recently proposed an expression for L at the limiting degenerate case,

$$\xi_{n(p)} \equiv \frac{E_{Fn(Fp)}(N^*, T)}{k_B T} \simeq 1, \text{ as: } L_{Kim}(|Sb|) = 1.5 + \exp\left[-\frac{|Sb|}{116}\right], \text{ } |Sb| \text{ being independent of } T \text{ or } N (?).$$

Then, being inspired from this $L_{Kim}(|Sb|)$ -expression, we also propose another one, given in the n(p)-type degenerate InP, as:

$$L_{VC}(|Sb(N^*, T)|) = 1.44296 + e^{-\frac{|Sb(N^*, T)|}{10^4}}; \quad |RD_{L, L_{VC}}| \equiv \left|1 - \frac{L_{VC}(|Sb(N^*, T)|)}{L}\right|, \quad (34)$$

where $|RD_{L, L_{VC}}|$ is the relative deviations in absolute values between L and L_{VC} .

Finally, the numerical results of above expressions are obtained and discussed in the following.

First, in the highly degenerate d(a)-InP, defined by physical conditions : $N = 10^{21} \text{ cm}^{-3}$ and $T (=3K \text{ and } 300K)$, the numerical results of $\xi_{n(p)} \equiv \frac{E_{Fn(Fp)}(N^*, T)}{k_B T}$, calculated by using Eq. (A3) of the Appendix A, and then

other ones of: $\sigma(N^*, r_{d(a)}, T)$ by Eq. (27), $\kappa(N^*, r_{d(a)}, T)$ by Eq. (25a); $C_\kappa(N^*, r_{d(a)})$, $\kappa_{App.}(N^*, r_{d(a)}, T)$ and $|RD_{\kappa, \kappa_{App.}}|_T$ by Eq. (25b), $Sb(N^*, T)$, $T_s(N^*, T)$, $P_t(N^*, T)$ and $ZT(N^*, T)$ by Equations (30, 31, 32, 33)

respectively, and finally, $|RD_{L, L_{VC}}|$ by Eq. (34), are obtained and reported in the following Tables 7 and 8.

Table 7. Here, one notes that (i) for a given T , with increasing r_d , due to the impurity size effect, $N_{CDn}(r_d)$, increases, since $N (=10^{21} \text{ cm}^{-3})$ is very high, N^* therefore decreases slowly, explaining the slow decrease (\searrow) in $\frac{E_{Fn}(N^*, T=300K)}{k_B T}$, σ , κ , C_κ , and $\kappa_{App.}$, (ii) the numerical result: $|RD_{\kappa, \kappa_{App.}}|_{300K} = 7.426 \times 10^{-5}$ confirms the $\kappa_{App.}$ -law, as given in Eq. (25b), and finally, (iii) $|RD_{L, L_{VC}}| = 1.534 \times 10^{-6}$ thus confirms in the degenerate InP -case the well-known Wiedemann-Frank, given in Eq. (25a), is found to be exact.

Donor	P	As	Te	Sb	Sn
Highly degenerate d-InP systems for $N=10^{21} \text{ cm}^{-3}$ and at $T=3K$ and $T=300K$, noting that $N^* \equiv N - N_{CDn}(r_d)$					
$\frac{E_{Fn}(N^*, T=300K)}{k_B T} \gg 1$	210.46	210.46	210.45	210.45	210.45
$\sigma_{(T=3K)} \left(\frac{10^6}{ohm \times cm}\right) \searrow$	1.2085	1.1552	0.8860	0.7979	0.7135
$\sigma_{(T=300K)} \left(\frac{10^6}{ohm \times cm}\right) \searrow$	1.2085	1.1553	0.8860	0.7979	0.7136

$\kappa_{(T=3K)} \left(\frac{10^{-2} \times W}{cm \times K} \right)$	\searrow	8.8567	8.4668	6.4933	5.8475	5.2295
$\kappa_{(T=300K)} \left(\frac{W}{cm \times K} \right)$	\searrow	8.8573	8.4674	6.4938	5.8479	5.2299
$C_{\kappa} \left(\frac{10^{-3} \times W}{cm \times K^2} \right)$	\searrow	29.522	28.222	21.6444	19.4917	17.4318
$\kappa_{App.} (300K) \left(\frac{W}{cm \times K} \right)$	\searrow	8.8567	8.4667	6.4933	5.8475	5.2295
$\left RD_{\kappa, \kappa_{App.}} \right _{300K}$ in 10^{-5}		7.426	7.426	7.426	7.426	7.426
$Sb_{(T=3K)} \left(\frac{10^{-8} \times V}{K} \right)$		-2.694	-2.694	-2.694	-2.694	-2.694
$Sb_{(T=300K)} \left(\frac{10^{-6} \times V}{K} \right)$		-2.694	-2.694	-2.694	-2.694	-2.694
$Ts_{(T=3K)} \left(\frac{10^{-8} \times V}{K} \right)$		-2.694	-2.694	-2.694	-2.694	-2.694
$Ts_{(T=300K)} \left(\frac{10^{-6} \times V}{K} \right)$		-2.693	-2.693	-2.693	-2.693	-2.693
$Pt_{(T=3K)} (10^{-8} \times V)$		-8.082	-8.082	-8.082	-8.082	-8.082
$Pt_{(T=300K)} (10^{-4} \times V)$		-8.081	-8.081	-8.081	-8.082	-8.082
$ZT_{(T=3K)} (\times 10^{-8})$		2.971	2.971	2.971	2.971	2.971
$ZT_{(T=300K)} (\times 10^{-4})$		2.970	2.970	2.970	2.970	2.971
<hr/>						
$ RD_{L, L_{VC}} $ in 10^{-6} at 3 K		1.534	1.534	1.534	1.534	1.534
$ RD $ in 10^{-6} at 300K		1.534	1.534	1.534	1.534	1.534

Table 8. Here, one notes that (i) for a given T, with increasing r_a , due to the impurity size effect, $N_{CDP}(r_a)$, increases, since $N(=10^{21} \text{ cm}^{-3})$ is very high, N^* therefore decreases slowly, explaining the slow decrease (\searrow) in $\frac{E_{FP}(N^*, T=300K)}{k_B T}$, σ , κ , C_{κ} , and $\kappa_{App.}$, (ii) the numerical result: $\left| RD_{\kappa, \kappa_{App.}} \right|_{300K} \simeq 4.788 \times 10^{-3}$ confirms the $\kappa_{App.}$ -law, as given in Eq. (25b), and finally, (iii) $|RD_{L, L_{VC}}| \simeq 1.535 \times 10^{-6}$ thus confirms in the degenerate InP-case the well-known Wiedemann-Frank, given in Eq. (25a), is found to be exact.

Acceptor		Ga (Al)	Mg	In
Highly degenerate a- InP systems for $N=10^{21} \text{ cm}^{-3}$ and $T=3K$ and $T=300K$				
$\frac{E_{FP}(N^*, T=300K)}{k_B T} \gg 1$	\searrow	28.21	28.21	28.21
$\sigma_{(T=3K)} \left(\frac{10^4}{ohm \times cm} \right)$	\searrow	3.52	3.15	3.13
$\sigma_{(T=300K)} \left(\frac{10^4}{ohm \times cm} \right)$	\searrow	3.54	3.16	3.15
$\kappa_{(T=3K)} \left(\frac{10^{-3} \times W}{cm \times K} \right)$	\searrow	2.5827	2.3106	2.2976
$\kappa_{(T=300K)} \left(\frac{W}{cm \times K} \right)$	\searrow	0.25934	0.2320	0.2307
$C_{\kappa} \left(\frac{10^{-3} \times W}{cm \times K^2} \right)$ at $T=3K$	\searrow	0.8609	0.7702	0.7658
$\kappa_{App.} (300K) \left(\frac{W}{cm \times K} \right)$	\searrow	0.25827	0.2311	0.2297
$\left RD_{\kappa, \kappa_{App.}} \right _{300K}$ in 10^{-3}		4.115	4.118	4.118
$Sb_{(T=3K)} \left(\frac{10^{-7} \times V}{K} \right)$		2.013	2.013	2.013
$Sb_{(T=300K)} \left(\frac{10^{-5} \times V}{K} \right)$		2.001	2.002	2.002
$Ts_{(T=3K)} \left(\frac{10^{-7} \times V}{K} \right)$		2.013	2.013	2.013

$Ts_{(T=300K)} \left(\frac{10^{-5} \times V}{K} \right)$	1.979	1.979	1.979
$Pt_{(T=3K)} (10^{-7} \times V)$	6.038	6.040	6.040
$Pt_{(T=300K)} (10^{-3} \times V)$	6.004	6.006	6.006
$ZT_{(T=3K)} (\times 10^{-6})$	1.658	1.659	1.659
$ZT_{(T=300K)} (\times 10^{-2})$	1.640	1.640	1.640
$ RD_{L,L_{VC}} $ in 10^{-6} at 3 K	1.534	1.534	1.534
$ RD_{L,L_{VC}} $ in 10^{-6} at 300 K	1.535	1.535	1.535

Secondly, in the degenerate d(a)-InP, for a given N^* , the values of $\xi_{n(p)} \equiv \frac{E_{Fn(Fp)}(N^*, T)}{k_B T}$, calculated by using Eq. (A3) of the Appendix A, and other ones of: $Sb(N^*, T)$ by Eq. (30), $|RD_{L,L_{VC}}|$ by Eq. (34), $ZT(N^*, T)$ by Eq. (33), and finally, $Ts(N^*, T)$ and $Pt(N^*, T)$ by Equations (31, 32), respectively, are obtained and reported in following Tables 9-11.

Table 9. Here, for a given N^* and for a given degenerate d-InP system, with increasing T , the reduced Fermi-energy ξ_n decreases, and other thermoelectric coefficients are in variations, as indicated by the arrows as: (\nearrow , \searrow). One notes that with increasing T : (i) for $\xi_n = 1.813$, while the numerical results of Sb present a same minimum $(Sb)_{\min.} \left(= -1.563 \times 10^{-4} \frac{V}{K} \right)$, those of ZT show a same maximum $ZT_{\max.} (= 1)$, (ii) for $\xi_n = 1$, Sb and ZT present same results: $-1.322 \times 10^{-4} \frac{V}{K}$ and 0.715, respectively, (iii) for $\xi_n = 1.813$ and $\xi_n = 1$, $(ZT)_{Mott} = \frac{\pi^2}{3 \times \xi_n^2}$ present same results: ≈ 1 and 3.290, respectively, and finally, (iv) the maximal value of $|RD_{L,L_{VC}}|$ is approximated to 1.541×10^{-6} , suggesting that in the degenerate InP -case the Wiedemann-Frank, given in Eq. (25a), is exact.

In the degenerate P- InP system, $N^* \equiv N - N_{CDn}(r_P) \equiv N_{CDn}(r_P)$; $N = 2N_{CDn}(r_P)$									
$T(K)$	\nearrow	5	10	21.814	25	29.384436	30		
ξ_n	\searrow	9.713	5.036	1.813	1.401	1	0.952		
$Sb \left(10^{-4} \frac{V}{K} \right)$		-0.564	\searrow -0.997	\searrow -1.563	\nearrow -1.512	\nearrow -1.322	\nearrow -1.296		
$ RD_{L,L_{VC}} $ in 10^{-6}		1.537	1.538	1.541	1.541	1.540	1.540		
ZT		0.130	\nearrow 0.406	\nearrow 1	\searrow 0.936	\searrow 0.715	\searrow 0.677		
$(ZT)_{Mott} = \frac{\pi^2}{3 \times \xi_n^2}$	\nearrow	0.035	0.130	0.9997	1.676	3.290	3.633		
$T_s \left(10^{-8} \frac{V}{K} \right)$		-5115	\searrow -7244	\nearrow -4.240	\nearrow 7183	\nearrow 16574	\nearrow 17819		
$Pt (10^{-3} V)$		-0.282	\searrow -0.997	\searrow -3.375	\searrow -3.781	\searrow -3.884	\nearrow -3.858		
In the degenerate As- InP system, $N^* \equiv N - N_{CDn}(r_{As}) \equiv N_{CDn}(r_{As})$; $N = 2N_{CDn}(r_{As})$									
$T(K)$	\nearrow	5	10	22.68	25	30.865609	31		
ξ_n	\searrow	10.189	5.273	1.813	1.533	1	0.990		
$Sb \left(10^{-4} \frac{V}{K} \right)$		-0.539	\searrow -0.961	\searrow -1.563	\nearrow -1.541	\nearrow -1.322	\nearrow -1.314		
$ RD_{L,L_{VC}} $ in 10^{-6}		1.537	1.538	1.541	1.541	1.540	1.540		
ZT		0.119	\nearrow 0.378	\nearrow 1	\searrow 0.972	\searrow 0.715	\searrow 0.707		
$(ZT)_{Mott} = \frac{\pi^2}{3 \times \xi_n^2}$	\nearrow	0.032	0.118	0.9996	1.399	3.290	3.358		
$T_s \left(10^{-8} \frac{V}{K} \right)$		-4935	\searrow -7079	\nearrow -4.973	\nearrow 4595	\nearrow 16574	\nearrow 16835		
$Pt (10^{-3} V)$		-0.270	\searrow -0.961	\searrow -3.545	\searrow -3.853	\searrow -4.079	\nearrow -4.075		
In the degenerate Te- InP system, $N^* \equiv N - N_{CDn}(r_{Te}) \equiv N_{CDn}(r_{Te})$; $N = 2N_{CDn}(r_{Te})$									
$T(K)$	\nearrow	5	10	30.2	35	41.089955	42		
ξ_n	\searrow	13.491	6.890	1.813	1.398	1	0.949		
$Sb \left(10^{-4} \frac{V}{K} \right)$		-0.413	\searrow -0.769	\searrow -1.563	\nearrow -1.511	\nearrow -1.322	\nearrow -1.284		
$ RD_{L,L_{VC}} $ in 10^{-6}		1.536	1.537	1.541	1.540	1.540	1.540		
ZT		0.070	\nearrow 0.242	\nearrow 1	\searrow 0.935	\searrow 0.715	\searrow 0.675		
$(ZT)_{Mott} = \frac{\pi^2}{3 \times \xi_n^2}$	\nearrow	0.018	0.069	1.0004	1.683	3.290	3.654		
$T_s \left(10^{-8} \frac{V}{K} \right)$		-3926	\searrow -6327	\nearrow 5.355	\nearrow 7247	\nearrow 16574	\nearrow 17889		
$Pt (10^{-3} V)$		-0.206	\searrow -0.769	\searrow -4.720	\searrow -5.290	\searrow -5.431	\nearrow -5.393		
In the degenerate Sb- InP system, $N^* \equiv N - N_{CDn}(r_{Sb}) \equiv N_{CDn}(r_{Sb})$; $N = 2N_{CDn}(r_{Sb})$									

T(K)	↗	5	10	33.84	35	46.6976	47
ξ_n	↘	15.10	7.677	1.813	1.713	1	0.952
Sb $(10^{-4} \frac{V}{K})$		-0.370	↘ -0.699	↘ -1.563	↗ -1.560	↗ -1.322	↗ -1.286
$ RD_{L,LVC} $ in 10^{-6}		1.536	1.537	1.541	1.541	1.540	1.540
ZT		0.056	↗ 0.200	↗ 1	↘ 0.997	↘ 0.715	↘ 0.677
$(ZT)_{Mott} = \frac{\pi^2}{3 \times \xi_n^2}$	↗	0.014	0.056	1.00003	1.120	3.290	3.628
Ts $(10^{-8} \frac{V}{K})$		-3557	↘ -5973	↗ 0.345	↗ 1511	↗ 16574	↗ 17803
Pt $(10^{-3}V)$		-0.185	↘ -0.699	↘ -5.289	↘ -5.461	↘ -6.086	↗ -6.047

In the degenerate Sn- InP system, $N^* \equiv N - N_{CDn}(r_{Sn}) \equiv N_{CDn}(r_{Sn})$; $N = 2N_{CDn}(Sn)$

T(K)	↗	5	10	38.165	45	51.928706	52
ξ_n	↘	17.005	8.616	1.813	1.353	1	0.997
Sb $(10^{-4} \frac{V}{K})$		-0.330	↘ -0.630	↘ -1.563	↗ -1.498	↗ -1.322	↗ -1.319
$ RD_{L,LVC} $ in 10^{-6}		1.536	1.537	1.541	1.540	1.540	1.540
ZT		0.044	↗ 0.162	↗ 1	↘ 0.919	↘ 0.715	↘ 0.713
$(ZT)_{Mott} = \frac{\pi^2}{3 \times \xi_n^2}$	↗	0.011	0.044	1.0003	1.797	3.290	3.311
Ts $(10^{-8} \frac{V}{K})$		-3194	↘ -5561	↗ 4.001	↗ 8191	↗ 16574	↗ 16657
Pt $(10^{-3}V)$		-0.165	↘ -0.630	↘ -5.965	↘ -6.742	↘ -6.863	↗ -6.861

Table 10. Here, for a given N^* and for a given degenerate a- InP system, with increasing T, the reduced Fermi-energy ξ_p decreases, and other thermoelectric coefficients are in variations, as indicated by the arrows as: (↗, ↘). One notes that with increasing T: (i) for $\xi_p = 1.813$, both Sb and ZT present same maximal results: $1.563 \times 10^{-4} \frac{V}{K}$ and 1, respectively, (ii) for $\xi_p = 1$, Sb and ZT present same results: $1.322 \times 10^{-4} \frac{V}{K}$ and 0.715, respectively, (iii) for $\xi_p = 1.813$ and $\xi_p = 1$, $(ZT)_{Mott} = \frac{\pi^2}{3 \times \xi_p^2}$ present same results: ≈ 1 and 3.290, respectively, and finally, (iv) the maximal value of $|RD_{L,LVC}|$ is approximated to 1.541×10^{-6} , suggesting that in the degenerate InP -case the Wiedemann-Frank, given in Eq. (25a), is exact.

In the degenerate Ga- InP system, $N^* \equiv N - N_{CDn}(r_{Ga}) \equiv N_{CDn}(r_{Ga})$; $N = 2N_{CDn}(r_{Ga})$							
T(K)	↗	5	10	54.15	65	73.687115	74
ξ_p	↘	24.08	12.12	1.813	1.307	1	0.990
Sb $(10^{-4} \frac{V}{K})$		0.234	↗ 0.458	↗ 1.563	↘ 1.483	↘ 1.322	↘ 1.315
$ RD_{L,LVC} $ in 10^{-6}		1.535	1.536	1.541	1.540	1.540	1.540
ZT		0.022	↗ 0.086	↗ 1	↘ 0.900	↘ 0.715	↘ 0.707
$(ZT)_{Mott} = \frac{\pi^2}{3 \times \xi_p^2}$	↗	0.006	0.022	0.99992	1.925	3.290	3.356
Ts $(10^{-8} \frac{V}{K})$		2305	↗ 4299	↘ 1.094	↘ -9185	↘ -16574	↘ -16829
Pt $(10^{-3}V)$		0.117	↗ 0.458	↗ 8.464	↗ 9.638	↗ 9.739	↘ 9.728

In the degenerate Mg- InP system, $N^* \equiv N - N_{CDn}(r_{Mg}) \equiv N_{CDn}(r_{Mg})$; $N = 2N_{CDn}(r_{Mg})$

T(K)	↗	5	10	61.99	65	84.343409	85
ξ_p	↘	27.54	13.841	1.813	1.673	1	0.982
Sb $(10^{-4} \frac{V}{K})$		0.205	↗ 0.403	↗ 1.563	↘ 1.558	↘ 1.322	↘ 1.309
$ RD_{L,LVC} $ in 10^{-6}		1.535	1.536	1.541	1.541	1.540	1.540
ZT		0.017	↗ 0.066	↗ 1	↘ 0.993	↘ 0.715	↘ 0.701
$(ZT)_{Mott} = \frac{\pi^2}{3 \times \xi_p^2}$	↗	0.004	0.017	1.0004	1.175	3.290	3.413
Ts $(10^{-8} \frac{V}{K})$		2025	↗ 3839	↘ -5.277	↘ -21555	↗ -16574	↘ -17040
Pt $(10^{-3}V)$		0.102	↗ 0.403	↗ 9.689	↗ 10.127	↗ 11.148	↘ 11.124

In the degenerate In- InP system, $N^* \equiv N - N_{CDn}(r_{In}) \equiv N_{CDn}(r_{In})$; $N = 2N_{CDn}(r_{In})$

T(K)	↗	5	10	62.34	65	84.831179	85
ξ_p	↘	27.705	13.920	1.813	1.690	1	0.995
Sb $(10^{-4} \frac{V}{K})$		0.204	↗ 0.400	↗ 1.563	↘ 1.559	↘ 1.322	↘ 1.318
$ RD_{L,LVC} $ in 10^{-6}		1.535	1.536	1.541	1.541	1.540	1.540
ZT		0.017	↗ 0.066	↗ 1	↘ 0.995	↘ 0.715	↘ 0.711
$(ZT)_{Mott} = \frac{\pi^2}{3 \times \xi_p^2}$	↗	0.004	0.017	0.99995	1.152	3.290	3.321
Ts $(10^{-8} \frac{V}{K})$		2014	↗ 3820	↘ 0.654	↘ -1885	↘ -16574	↘ -16694
Pt $(10^{-3}V)$		0.102	↗ 0.400	↗ 9.744	↗ 10.134	↗ 11.212	↘ 11.206

Table 11. Here, for a given N^* and for a given degenerate a- InP system, with increasing T , the reduced Fermi-energy ξ_p decreases, and other thermoelectric coefficients are in variations, as indicated by the arrows as: (\nearrow , \searrow). One notes that with increasing T : (i) for $\xi_p = 1.813$, both Sb and ZT present same maximal results: $1.563 \times 10^{-4} \frac{V}{K}$ and 1, respectively, (ii) for $\xi_p = 1$, Sb and ZT present same results: $1.322 \times 10^{-4} \frac{V}{K}$ and 0.715, respectively, (iii) for $\xi_p = 1.813$ and $\xi_p = 1$, $(ZT)_{Mott} = \frac{\pi^2}{3 \times \xi_p^2}$ present same results: ≈ 1 and 3.290, respectively, and finally, (iv) the maximal value of $|RD_{L,LVC}|$ is approximated to 1.541×10^{-6} , suggesting that in the degenerate InP -case the Wiedemann-Frank, given in Eq. (25a), is exact.

In the degenerate P- InP system, $N^* \equiv N - N_{CDn}(r_P) \equiv 2N_{CDn}(r_P)$; $N = 3N_{CDn}(r_P)$									
T(K)	\nearrow	5	10	34.283		40		46.644885	47
ξ_n	\searrow	15.29	7.772	1.813		1.380		1	0.982
Sb ($10^{-4} \frac{V}{K}$)		-0.366	\searrow -0.692	\searrow -1.563	\nearrow	-1.506	\nearrow	-1.322	\nearrow -1.309
$ RD_{L,LVC} $ in 10^{-6}		1.536	1.537	1.541		1.540		1.540	1.540
ZT		0.055	\nearrow 0.196	\nearrow 1	\searrow	0.929	\searrow	0.715	\searrow 0.701
$(ZT)_{Mott} = \frac{\pi^2}{3 \times \xi_n^2}$	\nearrow	0.014	0.054	1.0004		1.726		3.290	3.410
T_s ($10^{-8} \frac{V}{K}$)		-3517	\searrow -5931	\nearrow 5.707	\nearrow	7614	\nearrow	16574	\nearrow 17030
Pt ($10^{-3}V$)		-0.183	\searrow -0.692	\searrow -5.358	\searrow	-6.026	\searrow	-6.165	\nearrow -6.152
In the degenerate Sn- InP system, $N^* \equiv N - N_{CDn}(r_{Sn}) \equiv 2N_{CDn}(r_{Sn})$; $N = 3N_{CDn}(r_{Sn})$									
T(K)	\nearrow	5	10	60.58		70		82.431683	83
ξ_n	\searrow	26.92	13.532	1.813		1.406		1	0.984
Sb ($10^{-4} \frac{V}{K}$)		-0.210	\searrow -0.412	\searrow -1.563	\nearrow	-1.514	\nearrow	-1.322	\nearrow -1.310
$ RD_{L,LVC} $ in 10^{-6}		1.535	1.536	1.541		1.541		1.540	1.540
ZT		0.018	\nearrow 0.069	\nearrow 1	\searrow	0.938	\searrow	0.715	\searrow 0.703
$(ZT)_{Mott} = \frac{\pi^2}{3 \times \xi_n^2}$	\nearrow	0.004	0.018	1.0001		1.664		3.290	3.398
T_s ($10^{-8} \frac{V}{K}$)		-2070	\searrow -3915	\nearrow 1.730	\nearrow	7081	\nearrow	16574	\nearrow 16987
Pt ($10^{-3}V$)		-0.105	\searrow -0.412	\searrow -9.469	\searrow	-10.59	\searrow	-10.895	\nearrow -10.87
In the degenerate Ga(Al)- InP system, $N^* \equiv N - N_{CDn}(r_{Ga(Al)}) \equiv 2N_{CDn}(r_{Ga(Al)})$; $N = 3N_{CDn}(r_{Ga(Al)})$									
T(K)	\nearrow	5	10	85.95		90		116.971	117
ξ_p	\searrow	38.172	19.135	1.813		1.678		1	0.999
Sb ($10^{-4} \frac{V}{K}$)		0.148	\nearrow 0.294	\nearrow 1.563	\searrow	1.558	\searrow	1.322	\searrow 1.321
$ RD_{L,LVC} $ in 10^{-6}		1.535	1.536	1.541		1.541		1.540	1.540
ZT		0.009	\nearrow 0.035	\nearrow 1	\searrow	0.994	\searrow	0.715	\searrow 0.7146
$(ZT)_{Mott} = \frac{\pi^2}{3 \times \xi_p^2}$	\nearrow	0.002	0.009	0.99985		1.168		3.290	3.294
T_s ($10^{-8} \frac{V}{K}$)		1473	\nearrow 2865	\searrow 1.988	\searrow	-2080	\searrow	-16574	\searrow -16589
Pt ($10^{-3}V$)		0.074	\nearrow 0.294	\nearrow 13.435	\nearrow	14.025	\nearrow	15.460	\searrow 15.459
In the degenerate In- InP system, $N^* \equiv N - N_{CDn}(r_{In}) \equiv 2N_{CDn}(r_{In})$; $N = 3N_{CDn}(r_{In})$									
T(K)	\nearrow	5	10	98.96		99		134.6611	135
ξ_p	\searrow	43.936	22.010	1.813		1.812		1	0.994
Sb ($10^{-4} \frac{V}{K}$)		0.129	\nearrow 0.256	\nearrow 1.563	\searrow	1.5629	\searrow	1.322	\searrow 1.317
$ RD_{L,LVC} $ in 10^{-6}		1.535	1.535	1.541		1.541		1.540	1.540
ZT		0.007	\nearrow 0.027	\nearrow 1	\searrow	0.9999995	\searrow	0.715	\searrow 0.710
$(ZT)_{Mott} = \frac{\pi^2}{3 \times \xi_p^2}$	\nearrow	0.002	0.007	0.999998		1.001347		3.290	3.329
T_s ($10^{-8} \frac{V}{K}$)		1282	\nearrow 2511	\searrow 0.031	\searrow	-17.560	\searrow	-16574	\searrow -16725
Pt ($10^{-3}V$)		0.064	\nearrow 0.256	\nearrow 15.470	\nearrow	15.474	\nearrow	17.798	\searrow 17.786

In summary, from above Tables, for $\xi_{n(p)} \equiv \frac{E_{Fn(Fp)}(N^*, T)}{k_B T} \gtrsim 1$, the maximal value of $|RD_{L,LVC}|$ is equal to : 1.541×10^{-6} , suggesting that the above Wiedemann-Frank thermoelectric conversion law, given in Eq. (25a) is found to be exact, with the Lorenz number $L \equiv \frac{\pi^2}{3} \times \left(\frac{k_B}{q}\right)^2 = 2.4429637 \left(\frac{W \times ohm}{K^2}\right)$, even at the limiting degenerate case, $\xi_{n(p)} \approx 1$. In other word, our above $L_{VC}(N^*, T, r_{d(a)})$ -expression, given in Eq. (25b), is not useful in the present n(p)-type degenerate InP.

6. Concluding remarks

In the n(p)-type degenerate InP-crystal, by using the same physical model, as that given in Eq. (7), and same mathematical methods, as those proposed in Equations (14, 17, 22), and by taking into account the corrected values of energy-band-structure parameters, all the numerical results, obtained in II, are now revised and performed. So, by basing on our following basic expressions, as:

- (i) the effective extrinsic static dielectric constant, $\epsilon(r_{d(a)})$, due to the impurity size effect, determined by an effective Bohr model [1], and given in Eq. (2),
 - (ii) the critical donor(acceptor)-density, $N_{CDn(NDp)}(r_{d(a)})$, determined from the generalized effective Mott criterion in the MIT, and given in Eq. (3), being used to determine the effective d(a)-density: $N^* \equiv N - N_{CDn(CDp)}(r_{d(a)})$, which gives a physical condition, needed to define the metal-insulator transition (**MIT**) at $T=0K$, as: $N^* \equiv N - N_{CDn(CDp)}(r_{d(a)})=0$ or $N = N_{CDn(CDp)}(r_{d(a)})$,
 - (iii) the Fermi energy, $E_{Fn(Fp)}(N^*, T)$, determined in Eq. (A3) of the Appendix A, with a precision of the order of 2.11×10^{-4} [3], and finally,
 - (iv) the electrical conductivity, $\sigma(N^*, r_{d(a)}, T)$, the thermal conductivity, $\kappa(N^*, r_{d(a)}, T)$, and the Seebeck coefficient, $S_b(N^*, T)$, determined respectively in Equations (27, 25a, 30),
- we have investigated the optical, electrical, and thermoelectric properties. Then, some concluding remarks are discussed, and given in the following.

First of all, one notes that the MIT occurs in the degenerate case at $T=0K$ and $N^* = 0$, at which:

- (a) $E_{Fno(Fpo)}(N^* = 0) = 0$, determined by Eq. (A4) of the Appendix A, since it is proportional to $(N^*)^{2/3}$,
- (b) as discussed in Eq. (5), suggesting that, in the MIT,

$$E_{gn1(gp1)}(N^* = 0, r_{d(a)}, T = 0) = E_{gn2(gp2)}(N^* = 0, r_{d(a)}, T = 0) = E_{Fgni(Fgpi)}(r_{d(a)}),$$

where $E_{gn1(gp1)}$, $E_{gn2(gp2)}$ and $E_{Fgni(Fgpi)}$ are the optical band gap (OBG), reduced band gap and intrinsic band gap, respectively, and

- c) as discussed in Eq. (27) for the electrical conductivity, $\sigma(N^*, r_{d(a)}, T)$, which is proportional to $E_{Fno(Fpo)}^2$ or to $(N^*)^{4/3}$, giving rise to: $\sigma(N^* = 0, r_{d(a)}, T = 0) = 0$, and therefore, as discussed in Equations (28), (29) and (A7) of the Appendix A: $\mu(N^* = 0, r_{d(a)}, T = 0K) = 0$, $\mu_H(N^* = 0, r_{d(a)}, T = 0K) = 0$, and $D(N^* = 0, r_{d(a)}, T = 0K) = 0$.

Furthermore, for high N^* (or high N) and at low T , some concluding remarks are given as follows.

- (1) In Table 2, we remark that the maximal relative deviations, in absolute values, $|RD|$, between $N_{CDn(NDp)}(r_{d(a)})$ and $N_{CDn(CDp)}^{EBT}(r_{d(a)})$ are found to be equal to: $5.57(7.61) \times 10^{-4}$, respectively. In other word, the critical donor(acceptor)-density, $N_{CDn(NDp)}(r_{d(a)})$, determined in Eq. (3), can be used to explain the densities of electrons (holes) localized in exponential conduction (valance)-band (EBT) tails, $N_{CDn(CDp)}^{EBT}(r_{d(a)})$.

(2) In Tables 5 and 6, we remark that: **(i)** for given N and T , the functions: $\sigma(r_{d(a)})$, $\mu(r_{d(a)})$, $\mu_H(r_{d(a)})$ and $D(r_{d(a)})$, calculated using respective Equations (27, 28, 29, A8 of the Appendix A), decrease with increasing $r_{d(a)}$, and **(ii)** for given $r_{d(a)}$ and T , the functions: $\sigma(N^*)$ and $D(N^*)$ increase, while the functions: $\mu(N^*)$ and $\mu_H(N^*)$ decrease, with increasing N .

(3) In Tables 7 and 8, one notes that (i) for a given T , with increasing $r_{d(a)}$, due to the impurity size effect, $N_{CDn(CDp)}(r_{d(a)})$, increases, since $N(= 10^{21} \text{ cm}^{-3})$ is very high, N^* therefore decreases very slowly, explaining the slow decrease (\searrow) in $\frac{E_{Fn(Fp)}(N^*, T=300K)}{k_B T}$, σ , κ , C_κ , and $\kappa_{App.}$, **(ii)** the numerical results:

$\left| RD_{\kappa, \kappa_{App.}} \right|_{300K} \simeq 7.426 \times 10^{-5} (4.118 \times 10^{-3})$, respectively, confirm the $\kappa_{App.}$ -law, as that given in Eq. (25b), and finally, **(iii)** $\left| RD_{L, L_{VC}} \right| \simeq 1.5 \times 10^{-6}$ thus confirms in the degenerate InP-case the well-known Wiedemann-Frank law, given in Eq. (25a), is found to be exact.

(4) In Tables 9-11, for a given $N \geq 2N_{CDn(NDp)}$ or $N^* \geq N_{CDn(NDp)}$ and for a given degenerate d(a)-InP system, with increasing T , the reduced Fermi-energy $\xi_{n(p)}$ decreases, and other thermoelectric coefficients are in variations, as indicated by the arrows as: (\nearrow , \searrow). One notes here that with increasing T : **(i)** for $\xi_{n(p)} = 1.813$, while the values of Sb present a same minimum (maximum) $(Sb)_{\min.(\max.)} (= (\mp) 1.563 \times 10^{-4} \frac{V}{K})$, those of ZT show a same maximum $ZT_{\max.} (= 1)$, **(ii)** for $\xi_n = 1$, those of Sb and those of ZT present same results: $Sb (= (\mp) 1.322 \times 10^{-4} \frac{V}{K})$ and 0.715, respectively, **(iii)** for $\xi_n = 1.813$ and $\xi_n = 1$, those of $(ZT)_{Mott} = \frac{\pi^2}{3 \times \xi_{n(p)}^2}$ present same results: $\simeq 1$ and 3.290, respectively, and finally, **(iv)** the maximal value of $\left| RD_{L, L_{VC}} \right|$ is equal approximately to 1.541×10^{-6} , suggesting that in the degenerate InP-case the Wiedemann-Frank law, given in Eq. (25a), is exact, with the Lorenz number $L \equiv \frac{\pi^2}{3} \times \left(\frac{k_B}{q} \right)^2 = 2.4429637 \left(\frac{W \times ohm}{K^2} \right)$, even at the limiting degenerate case, $\xi_{n(p)} \simeq 1$. Therefore, our above $L_{VC}(N^*, T, r_{d(a)})$ -expression, given in Eq. (25b), is found to be not useful in the present degenerate n(p)-type InP.

In summary, all the numerical results, given in II [2], are now revised and performed in the present work.

Appendix

Appendix A. Fermi Energy and generalized Einstein relation

A1. In the n(p)-type InP-crystals, the Fermi energy $E_{Fn(Fp)} \equiv [E_{fn} - E_c](E_{Fp} \equiv [E_v - E_{fp}])$, $E_{c(v)}$ being the conduction (valence) band edges, obtained for any T and donor (acceptor) density N , being investigated in our previous paper, with a precision of the order of 2.11×10^{-4} [3], is now summarized in the following. In this work, N is replaced by the effective density N^* , $N^* \equiv N - N_{CDn(CDp)}(r_{d(a)})$, $N_{CDn(CDp)}(r_{d(a)})$ being

the critical density, characteristic of the insulator-metal transition (**MIT**) phenomenon. It means that $N^* = 0$ at this transition.

First of all, we define the reduced electron density by:

$$u(N^*, r_{d(a)}, T) \equiv u(N^*, T) \equiv \frac{N^*}{N_{c(v)}}, N_{c(v)}(T) = 2 \times g_{c(v)} \times \left(\frac{m_{n(p)}^* \times k_B T}{2\pi\hbar^2} \right)^{\frac{3}{2}} \text{ (cm}^{-3}\text{)}, \quad (\text{A1})$$

where $N_{c(v)}(T)$ is the conduction (valence)-band density of states, and the values of $g_{c(v)}$ and $m_{n(p)}^*$ are defined and given in Table 1. Then, the reduced Fermi energy in the n(p)-type InP is determined by :

$$\frac{E_{Fn}(u)}{k_B T} \left(\frac{E_{Fp}(u)}{k_B T} \right) = \frac{G(u) + Au^B F(u)}{1 + Au^B} = \theta_n(u) \equiv \frac{V(u)}{W(u)}, A = 0.0005372 \text{ and } B = 4.82842262, \quad (\text{A2})$$

where $F(N^*, r_{d(a)}, T) = au^{\frac{2}{3}} \left(1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}} \right)^{-\frac{2}{3}}$, obtained for $u \gg 1$, according to the degenerate cas,

$a = [(3\sqrt{\pi}/4)]^{2/3}$, $b = \frac{1}{8} \left(\frac{\pi}{a} \right)^2$, $c = \frac{62.3739855}{1920} \left(\frac{\pi}{a} \right)^4$, and then $G(u) \simeq \text{Ln}(u) + 2^{-\frac{3}{2}} \times u \times e^{-du}$ for $u \ll 1$, according to the non – degenerate case, with: $d = 2^{3/2} \left[\frac{1}{\sqrt{27}} - \frac{3}{16} \right] > 0$.

So, in the present degenerate case ($u \gg 1$), one has:

$$E_{Fn(Fp)}(N^*, r_{d(a)}, T) \equiv E_{Fn(Fp)}(N^*, T) = E_{Fn0(Fp0)}(u) \times \left(1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}} \right)^{-\frac{2}{3}}. \quad (\text{A3})$$

Then, at $T=0K$, since $u^{-1} = 0$, Eq. (A.3) is reduced to:

$$E_{Fn0(Fp0)}(N^*) \equiv \frac{\hbar^2 \times k_{Fn(Fp)}^2(N^*)}{2 \times m_{n(p)}^*}, \quad (\text{A4})$$

being proportional to $(N^*)^{2/3}$, and equal to 0, $E_{Fn0(Fp0)}(N^* = 0) = 0$, according to the MIT, as discussed in Section 2 and 3.

A2. Now, the generalized Einstein relation is defined by:

$$\frac{D(N^*, r_{d(a)}, T)}{\mu(N^*, r_{d(a)}, T)} \equiv \frac{N}{q} \times \frac{dE_{Fn(Fp)}}{dN} \equiv \frac{k_B \times T}{q} \times \left(u \frac{d\theta_n(p)}{du} \right), \quad (\text{A5})$$

where $\theta_n(u)$ is defined in (A2) and the mobility $\mu(N^*, r_{d(a)}, T)$ is determined in Eq. (28). Then, by differentiating this function $\theta_n(u)$ with respect to u , one thus obtains $\frac{d\theta_n}{du}$. Therefore

$$\frac{D(N^*, r_{d(a)}, T)}{\mu(N^*, r_{d(a)}, T)} = \frac{k_B \times T}{q} \times u \frac{V'(u) \times W(u) - V(u) \times W'(u)}{W^2(u)}, \quad (\text{A6})$$

where $W'(u) = ABu^{B-1}$ and $V'(u) = u^{-1} + 2^{-\frac{3}{2}} e^{-du}(1 - du) + \frac{2}{3} Au^{B-1} F(u) \left[\left(1 + \frac{3B}{2} \right) + \frac{4}{3} \times \frac{bu^{-\frac{4}{3}} + 2cu^{-\frac{8}{3}}}{1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}}} \right]$. One

remarks that: (i) as $u \rightarrow 0$, one has: $W^2 \simeq 1$ and $u[V' \times W - V \times W'] \simeq 1$, and therefore: $\frac{D_{n(p)}(u)}{\mu} \simeq \frac{k_B \times T}{q}$,

and (ii) as $u \rightarrow \infty$, one has: $W^2 \approx A^2 u^{2B}$ and $u[V' \times W - V \times W'] \approx \frac{2}{3} au^{2/3} A^2 u^{2B}$, and therefore, in this highly degenerate case and at $T=0K$,

$$\frac{D(N^*, r_{d(a)}, T=0)}{\mu(N^*, r_{d(a)}, T=0)} \approx \frac{2}{3} E_{Fn0(Fp0)}(N^*)/q. \quad (\text{A.7})$$

One notes that, for $N^* = 0$, $\mathbb{E}_{\text{Fno}(\text{Fpo})}(N^*) = 0$, as remarked in above Eq. (A4), $\mu(N^* = 0, r_{d(a)}, T = 0K) = 0$, as remarked in above Eq. (28), and therefore, for any $r_{d(a)}$, $D(N^* = 0, r_{d(a)}, T = 0K) = 0$, according to the MIT. Now, replacing $\mathbb{E}_{\text{Fno}(\text{Fpo})}$ given in Eq. (A.7) by $\mathbb{E}_{\text{Fn}(\text{Fp})}$ determined in Eq. (A.3), Eq. (A.7) thus becomes in the present degenerate case, as

$$\frac{D(N^*, r_{d(a)}, T=0)}{\mu(N^*, r_{d(a)}, T=0)} \simeq \frac{2}{3} \times \mathbb{E}_{\text{Fno}(\text{Fpo})}(u) \times \left(1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}}\right)^{-\frac{2}{3}}. \quad (\text{A.8})$$

Appendix B. Approximate forms for band gap narrowing (BGN)

First of all, in the n(p)-type InP-crystals, we define the effective reduced Wigner-Seitz radius $r_{\text{sn}(\text{sp})}$, characteristic of the interactions, by:

$$r_{\text{sn}(\text{sp})}(N^*, r_{d(a)}) \equiv \left(\frac{3g_{c(v)}}{4\pi N^*}\right)^{1/3} \times \frac{1}{a_{\text{Bn}(\text{Bp})}(r_{d(a)})} = 1.1723 \times 10^8 \times \left(\frac{g_{c(v)}}{N^*}\right)^{1/3} \times \frac{m_{n(p)}^*/m_0}{\varepsilon(r_{d(a)})}. \quad (\text{B1})$$

Here, the values of $g_{c(v)} = 1(1)$ and $(m_{n(p)}^*/m_0)$ are defined and given in Table 1.

In particular, in the following, $m_{n(p)}^*/m_0 = m_r/m_0$, is taken for evaluating the band gap narrowing (BGN), as used in Section 3. Therefore, the correlation energy of an effective electron gas, $\mathbb{E}_{\text{CE}}(r_{\text{sn}(\text{sp})})$, is found to be given by [1]:

$$\mathbb{E}_{\text{CE}}(r_{\text{sn}(\text{sp})}) \equiv \mathbb{E}_{\text{CE}}(N^*, r_{d(a)}) = \frac{-0.87553}{0.0908 + r_{\text{sn}(\text{sp})}} + \frac{\frac{0.87553}{0.0908 + r_{\text{sn}(\text{sp})}} + \left(\frac{2[1 - \ln(2)]}{\pi^2}\right) \times \ln(r_{\text{sn}(\text{sp})}) - 0.093288}{1 + 0.03847728 \times r_{\text{sn}(\text{sp})}^{1.67378876}}. \quad (\text{B2})$$

Then, the band gap narrowing (BGN) can be determined by [1]:

$$\Delta \mathbb{E}_{\text{gn}}(N^*, r_d) \simeq a_1 \times \frac{\varepsilon_0}{\varepsilon(r_d)} \times N_r^{1/3} + a_2 \times \frac{\varepsilon_0}{\varepsilon(r_d)} \times N_r^{1/3} \times (2.503 \times [-\mathbb{E}_{\text{CE}}(r_{\text{sn}}) \times r_{\text{sn}}]) + a_3 \times \left[\frac{\varepsilon_0}{\varepsilon(r_d)}\right]^{5/4} \times \sqrt{\frac{m_v}{m_r}} \times N_r^{1/4} + a_4 \times \sqrt{\frac{\varepsilon_0}{\varepsilon(r_d)}} \times N_r^{1/2} \times 2 + a_5 \times \left[\frac{\varepsilon_0}{\varepsilon(r_d)}\right]^3 \times N_r^{1/6}, \quad (\text{B3})$$

$$N_r \equiv \frac{N^* = N - N_{\text{CDn}}(r_d)}{9.999 \times 10^{17} \text{ cm}^{-3}},$$

where $a_1 = 6.829 \times 10^{-3}(\text{eV})$, $a_2 = 1.168 \times 10^{-3}(\text{eV})$, $a_3 = 5.032 \times 10^{-3}(\text{eV})$, $a_4 = 10.058 \times 10^{-3}(\text{eV})$ and $a_5 = 1.455 \times 10^{-3}(\text{eV})$, and

$$\Delta \mathbb{E}_{\text{gp}}(N^*, r_a) \simeq a_1 \times \frac{\varepsilon_0}{\varepsilon(r_a)} \times N_r^{1/3} + a_2 \times \frac{\varepsilon_0}{\varepsilon(r_a)} \times N_r^{1/3} \times (2.503 \times [-\mathbb{E}_{\text{CE}}(r_{\text{sp}}) \times r_{\text{sp}}]) + a_3 \times \left[\frac{\varepsilon_0}{\varepsilon(r_a)}\right]^{5/4} \times \sqrt{\frac{m_c}{m_r}} \times N_r^{1/4} + 2a_4 \times \sqrt{\frac{\varepsilon_0}{\varepsilon(r_a)}} \times N_r^{1/2} + a_5 \times \left[\frac{\varepsilon_0}{\varepsilon(r_a)}\right]^3 \times N_r^{1/6}, \quad (\text{B4})$$

$$N_r \equiv \left(\frac{N^* = N - N_{\text{CDp}}(r_a)}{9.999 \times 10^{17} \text{ cm}^{-3}}\right),$$

where $a_1 = 9.329 \times 10^{-3}(\text{eV})$, $a_2 = 1.596 \times 10^{-3}(\text{eV})$, $a_3 = 7.144 \times 10^{-3}(\text{eV})$, $a_4 = 13.741 \times 10^{-3}(\text{eV})$ and $a_5 = 1.988 \times 10^{-3}(\text{eV})$.

Therefore, in Equations (B3, B4), as $N^* = 0$, and for any r_a , $\Delta \mathbb{E}_{\text{gn}(\text{gp})}(N^* = 0, r_a) = 0$, according to the MIT.

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