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Same maximum figure of merit ZT(=1), due to the effect of impurity size, obtained in the n(p)-type degenerate GaSb-crystal ($\xi_{n(p)}(\geqq 1)$), at same reduced Fermi energy $\xi_{n(p)}(=1.814)$, same minimum Seebeck coefficient $S\left(=-1.563\times10^{-4}\frac{V}{K}\right)$, and same $(ZT)_{Mott}\left(=\frac{\pi^2}{3\times\xi_{n(p)}^2}\simeq 1\right)$

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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, $\varepsilon(r_{d(a)})$, $r_{d(a)}$ 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 the n(p)-type degenerate GaSb-crystal, defined for the reduced Fermi energy $\xi_{n(p)}(\geqq 1)$. 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 9-10, with a given d(a)-density N $[=1.1\ (2)\times N_{CDn(NDp)}(r_{d(a)})]$, one notes here that with increasing temperature T(K): **(i)** for reduced Fermi energy $\xi_{n(p)}(=1.814)$, while the numerical results of the Seebeck coefficient S present a same minimum $\left(=-1.563\times10^{-4}\frac{V}{K}\right)$, those of the figure of merit ZT

show a same maximum $ZT(=\mathbf{1})$, **(ii)** for $\xi_n = 1$, those of S and ZT present same results: $Sb(=-1.322\times 10^{-4}\frac{V}{K})$ and 0.715, respectively, **(iii)** for $\xi_{n(p)} = 1.814$ and $\xi_{n(p)} = 1$, those of the well-known Mott figure of merit give same $(ZT)_{Mott} = \frac{\pi^2}{3\times\xi_{n(p)}^2}$ ($\simeq 1$ and 3.29), respectively, and finally, **(iv)** we show here that in the degenerate GaSb-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], $\boldsymbol{\xi_{n(p)}}(\geqq \mathbf{1})$. 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] 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 4-10. Finally, some concluding remarks are given in Section 6.

2. Energy-band-structure parameters

First of all, in the following Table 1, we present the values of the energy-band-structure parameters, given in the n(p)-type GaSb -crystals, such as: (i) if denoting the free electron mass by m_o, the effective electron (hole) mass, $m^*_{n(p)}/m_o$, which is respectively equal to the relative effective mass, $m_{n(p)}/m_o = 0.047$ (0.3) [5], as used in this Sections 2 and 4 to determine the critical impurity density in the metal-insulator transition (**MIT**), and (ii) to the reduced effective mas, $m_r/m_o = \frac{m_n\times m_p}{m_n+m_p} = 0.040634$, as used in Sections 3 and 5 to determine the optical band gap and the optical coefficients given in the n(p)-type

heavily doped InAs-crystals. Further, $E_{go}= E_{gGaSb}= E_{gSb}= E_{gGa} = 0.81$ eV [4] is the unperturbed intrinsic band gap, $\varepsilon_{GaSb}= \varepsilon_{Ga} = \varepsilon_{Sb} = \varepsilon_o = 15.69$ is the relative static intrinsic dielectric constant of the GaSb-crystal, and finally, the effective averaged numbers of equivalent conduction (valence)-band edge, $g_{c(v)} = 1(1)$.

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

$m_{n(p)}/m_o$ [4]	m_r/m_o	$m_{Cn(Cp)}/m_o$	$g_{c(v)}$	E_{go} [4]	ε_o [4]
0.047 (0.3)	0.0406	0.06 (0.4)	1(1)	0.81 eV	15.69

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

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

In the [d(a)-GaSb]-systems, since $r_{d(a)}$, given in tetrahedral covalent bonds, is usually either larger or smaller than $r_{Sb(Ga)} = 0.136\, nm$ $(0.126\, nm)$, a local mechanical strain (or deformation potential energy) is induced, according to a compression (dilation) for: $r_{d(a)} > r_{As(In)}$ $(r_{d(a)} < r_{As(In)})$, due to the d(a)-size effect, respectively [1, 2]. Then, we have shown that this $r_{d(a)}$-effect affects the changes in all the energy-band-structure parameters, expressed in terms of the static dielectric constant, $\varepsilon(r_{d(a)})$, determined as follows.

At T=0K, we have showed [1, 2] that such the compression (dilatation) corresponds to the repulsive (attractive) force increases (decreases) the intrinsic energy gap $E_{gni(gpi)}(r_{d(a)})$ and the effective donor(acceptor)-ionization energy $E_{d(a)}(r_{d(a)})$ in absolute values, obtained in an effective Bohr model, as:

$$E_{gni(gpi)}(r_{d(a)}) - E_{go} = E_{d(a)}(r_{d(a)}) - E_{do(ao)} = E_{do(ao)} \times \left[\left(\frac{\varepsilon_o}{\varepsilon(r_{d(a)})}\right)^2 - 1\right], \quad (1)$$

where $E_{do(ao)} \equiv \frac{13600\ \text{meV}\times(m_{n(p)}/m_o)}{\varepsilon_o^2} = 2.5965$ meV (16.57 meV), and

$$\varepsilon(r_{d(a)}) = \frac{\varepsilon_o}{\sqrt{1+\left[\left(\frac{r_{d(a)}}{r_{Sb(Ga)}}\right)^3 - 1\right]\times \ln\left(\frac{r_{d(a)}}{r_{Sb(Ga)}}\right)^3}} \leq \varepsilon_o, \text{ for } r_{d(a)} \geq r_{Sb(Ga)},$$

$$\varepsilon(r_{d(a)}) = \frac{\varepsilon_o}{\sqrt{1-\left[\left(\frac{r_{d(a)}}{r_{Sb(Ga)}}\right)^3 - 1\right]\times \ln\left(\frac{r_{d(a)}}{r_{Sb(Ga)}}\right)^3}} \geq \varepsilon_o, \left[\left(\frac{r_{d(a)}}{r_{Sb(Ga)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{Sb(Ga)}}\right)^3 < 1, \text{ for } r_{d(a)} \leq r_{Sb(Ga)}. \quad (2)$$

2.2. Our expressions for the critical density in the MIT

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

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

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

$$a_{Bn(Bp)}(r_{d(a)}) \equiv \frac{\varepsilon(r_{d(a)})\times\hbar^2}{m^*_{n(p)}\times q^2} = 0.53\times10^{-8}\ \text{cm}\times\frac{\varepsilon(r_{d(a)})}{(m^*_{n(p)}/m_o)}, \quad (4)$$

where $-q$ is the electron charge, $\varepsilon(r_{d(a)})$ is determined in Eq. (2), in which $m^*_{n(p)}/m_o = m_{n(p)}/m_o = 0.047\ (0.3)$. Here, we have chosen, in this work, y=1.6425 (0.25732) so that we obtain: $N_{CDn(NDp)}(r_{Sb(Ga)}) = 8\times10^{17}\ \text{cm}^{-3}$ [4]. Then, from Eq. (3), the numerical results of $N_{CDn(NDp)}(r_{d(a)})$ are obtained and given in the following Table 2, in which we also report those of the densities of electrons (holes), being localized in exponential conduction (valance)-band (EBT) tails, $N^{EBT}_{CDn(CDp)}(r_{d(a)})$, obtained using the next Eq. (21), as investigated in Section 4, noting that the maximal relative deviations (RD), in absolute values, between $N_{CDn(NDp)}(r_{d(a)})$ and $N^{EBT}_{CDn(CDp)}(r_{d(a)})$ are found to be equal to: 7.8% (5.9%), respectively. Thus, the numerical results of $N_{CDn(NDp)}(r_{d(a)})$ are obtained, using Eq. (3), can be explained by the densities of electrons (holes) localized in exponential conduction (valance)-band (EBT) tails, $N^{EBT}_{CDn(CDp)}(r_{d(a)})$, being determined from Eq. (21).

Table 2. For increasing $r_{d(a)}$, while $\varepsilon(r_{d(a)})$ decreases, the functions: $\mathbb{E}_{gni(gpi)}(r_{d(a)})$, $N_{CDn(NDp)}(r_{d(a)})$ and $N^{EBT}_{CDn(CDp)}(r_{d(a)})$ increase. The maximal relative deviations between the numerical results of $N_{CDn(NDp)}(r_{d(a)})$ and $N^{EBT}_{CDn(CDp)}(r_{d(a)})$, in absolute values, calculated using Equations (3, 21), are found to be equal to: 7.8% (5.9)%, respectively, suggesting that $N_{CDn(NDp)}(r_{d(a)})$ can be explained by $N^{EBT}_{CDn}(r_d)$, being localized in the EBT. So, in the n(p)-type GaSb- crystal, in which $(m_{n(p)}/m_o) = 0.047\ (0.3)$ [4], all the numerical results for the energy-band-structure parameters and $N_{CDn(CDp)}(r_{d(a)})$, which are expressed as functions of $r_{d(a)}$-radius, are obtained, using Equations (3, 9, 10, 11, 12, 13, 21).

Donor		P	As	Te	Sb	Sn
r_d (nm) [4]	↗	0.110	0.118	0.132	0.136	0.140
$\varepsilon(r_d)$	↘	18.7494	16.9954	15.7505	15.69	15.6284
$E_d(r_d)$ in meV	↗	1.8183	2.2130	2.5766	2.5965	2.6170
$E_{gni}(r_d)$ in eV	↗	0.8092	0.8096	0.80998	0.81	0.81002
$N_{CDn}(r_d)$ in $10^{17}\ \text{cm}^{-3}$	↗	4.6883	6.2949	7.9085	8	8.0954
$N^{EBT}_{CDn}(r_d)$ in $10^{17}\ \text{cm}^{-3}$	↗	5.0549	6.2463	7.3636	7.4250	7.4890
|RD|		**7.8%**	0.77%	6.9%	7.2%	7.5%
$R_{sn} < 1$, from Eq. (7),	↘	0.0134	0.0123	0.0115	0.0114	0.0114

Acceptor		Ge	Ga(Al, Mn)	Mg	In
r_a (nm) [4]	↗	0.122	0.126	0.140	0.144
$\varepsilon(r_a)$	↘	15.7605	15.69	14.8422	14.3386
$E_a(r_a)$ in meV	↗	16.48	16.57	18.52	19.84
$E_{gpi}(r_a)$ in eV	↗	0.8098	0.81	0.8119	0.8133
$N_{CDp}(r_a)$ in $10^{17}\ \text{cm}^{-3}$	↗	7.8931	8	9.4507	10.4818
$N^{EBT}_{CDp}(r_a)$ in $10^{17}\ \text{cm}^{-3}$	↗	8.3576	8.4232	9.2832	9.8655
|RD|		**5.9%**	5.35%	1.8%	5.88%
$R_{sp} < 1$, from Eq. (7),	↘	0.4581	0.4575	0.4490	0.4436

In summary, Table 2 also indicates that, for an increasing $r_{d(a)}$, $\varepsilon(r_{d(a)})$ decreases, while $E_{gni(gpi)}(r_{d(a)})$, $N_{CDn(NDp)}(r_{d(a)})$ and $N^{EBT}_{CDn(CDp)}(r_{d(a)})$ increase, affecting strongly all the physical properties, as those observed in following Sections 3-5 .

3. Optical band gap

Here, $m^*_{n(p)}/m_o$ is chosen as: $m^*_{n(p)}/m_o = m_r/m_o = 0.040634$, and then, if denoting $N^* \equiv N - N_{CDn(NDp)}(r_{d(a)})$, the optical band gap (**OBG**) is found to be given by:

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

where the Fermi energy $E_{Fn(Fp)}(N^*, T)$ is determined in Eq. (A3) of the Appendix A and the reduced band gap is defined by:

$$E_{gn2(gp2)}(N^*, r_{d(a)}, T) \equiv E_{gnei(gpei)}(r_{d(a)}, T) - \Delta E_{gn(gp)}(N^*, r_{d(a)}).$$

Here, the effective intrinsic band gap $\mathbb{E}_{gnei(gpei)}$ is determined by:

$$E_{gnei(gpei)}(r_{d(a)}, T) \equiv E_{gni(gpi)}(r_{d(a)}) - 0.20251\ eV \times \left(\left[1 + \left(\frac{2T}{440.0613\ K} \right)^{2.201} \right]^{\frac{1}{2.201}} - 1 \right),$$

and the band gap narrowing, $\Delta E_{gn(gp)}(N^*, r_{d(a)})$, are determined in Equations (B3, B4) of the Appendix B and the values of $E_{gni(gpi)}(r_{d(a)})$ are given in Table 1. In particular, in the n(p)-type Sb(Ga)-GaSb crystals, one gets: $E_{gnei(gpei)}(r_{Sb(Ga)}, T = 300\ K)$= 0.68 eV [4].

Further, as noted in the Appendix A and B, at T=0K, as $N^* = 0$, one has: $E_{Fn(Fp)}(N^*, T) = E_{Fno(Fpo)}(N^*) = 0$, as given in Eq. (A4), and $\Delta E_{gn(gp)}(N^*, r_{d(a)}) = 0$, according to the MIT, as noted in Appendix A and B. Therefore, $E_{gn1(gp1)} = E_{gn2(gp2)} = E_{gnei(gpei)}(r_{d(a)}) = E_{gni(gpi)}(r_{d(a)})$ at T=0K and $N^* = 0$, according also to the MIT.

Then, in degenerate d(a)- GaSb systems at T=20K, the numerical results of the OBG, evaluated using Eq. (5), are reported in the following Table 3, suggesting that, for a given $r_{d(a)}$, the OBG increases with increasing N.

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

N (10^{18} cm^{-3}) ↗	4	8.5	15	50	80
$\mathbb{E}_{gn1}(N^*, r_P)$ in eV ↗	0.983	1.122	1.283	1.917	2.343
$\mathbb{E}_{gn1}(N^*, r_{As})$ in eV ↗	0.975	1.114	1.275	1.908	2.333
$\mathbb{E}_{gn1}(N^*, r_{Te})$ in eV ↗	0.968	1.107	1.268	1.900	2.324
$\mathbb{E}_{gn1}(N^*, r_{Sb})$ in eV ↗	0.967	1.107	1.268	1.899	2.323
$\mathbb{E}_{gn1}(N^*, r_{Sn})$ in eV ↗	0.966	1.106	1.267	1.899	2.323

N (10^{18} cm^{-3}) ↗	6.5	11	15	26	60
$\mathbb{E}_{gp1}(N^*, r_{Ga(Al)})$ in eV ↗	1.056	1.181	1.277	1.505	2.061

$\mathbb{E}_{gp1}(N^*, r_{Mg})$ in eV	↗	1.052	1.177	1.273	1.501	2.057
$\mathbb{E}_{gp1}(N^*, r_{In})$ in eV	↗	1.049	1.174	1.271	1.499	2.054

4. Physical model and mathematical methods

4.1. Physical model

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

$$\gamma \times r_{sn(sp)}\left(N^*, r_{d(a)}, m^*_{n(p)}\right) \equiv \frac{k^{-1}_{Fn(Fp)}}{a_{Bn(Bp)}} < 1, \tag{6}$$

being proportional to $N^{*-1/3}$. Here, $\gamma = (4/9\pi)^{1/3}$, $k^{-1}_{Fn(Fp)}$ 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

$$R_{sn(sp)}\left(N^*, r_{d(a)}\right) \equiv \frac{k_{sn(sp)}}{k_{Fn(Fp)}} = \frac{k^{-1}_{Fn(Fp)}}{k^{-1}_{sn(sp)}} = a \times R_{snWS(spWS)} + \left[b \times R_{snTF(spTF)} - a \times R_{snWS(spWS)}\right] e^{-r_{sn(sp)}} < 1, \tag{7}$$

where the empirical parameters: $a = 0.068\ (0.7615)$ and b= 0 (0), respectively, were chosen so that the relative deviations between $N_{CDn(NDp)}$ and $N^{EBT}_{CDn(CDp)}$, in absolute values, are minimized, as observed in Table 1. Here, 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 $R_{snTF(spTF)}\left(N^*, r_{d(a)}\right)$ is reduced to

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

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

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

$$R_{sn(sp)WS}\left(N^*, r_{d(a)}\right) \equiv \frac{k_{sn(sp)WS}}{k_{Fn}} = \left(\frac{3}{2\pi} - \gamma \frac{d\left[r^2_{sn(sp)} \times \mathbb{E}_{CE}\left(N^*, r_{d(a)}\right)\right]}{dr_{sn(sp)}}\right), \tag{9}$$

where $\mathbb{E}_{CE}\left(N^*, r_{d(a)}\right)$ is the majority-carrier correlation energy (CE), being determined in Eq. (B2) of the Appendix B.

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

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

being needed to determine the expression for optical coefficients, as those investigated in Section 5. Here, $R_{sn(sp)}$ is defined in Eq. (7). Here, the energy parameter, $\eta_{n(p)}$, being characteristic of the exponential conduction (valence)-band tails is determined in next Eq. (12).

Then, in degenerate d(a)- GaSb 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 $\overrightarrow{R_j}$, randomly distributed throughout the GaSb -crystal, is defined by

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

where $\mathbb{N}$ 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)- GaSb system, defined as

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

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 $\vec{k}$-espace is given by

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

where Ω is the total GaSb -crystal volume.

Then, the effective auto-correlation function for potential fluctuations, $W_{n(p)}(\nu_{n(p)}, N^*, r_d) \equiv \langle V(r)V(r')\rangle$, was determined as [3] :

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

Here, $\varepsilon(r_{d(a)})$ is determined in Eq. (2), $R_{sn(sp)}(N^*, r_{d(a)})$in Eq. (7), the empirical Heisenberg parameter $\mathcal{H} = 0.1\ (0.1\ )$, respectively, will be chosen such that the determination of the density of electrons localized in the conduction(valence)-band tails, determined in Section 5 would be accurate, and finally $\nu_{n(p)} \equiv \frac{-\mathbb{E}}{\mathbb{E}_{Fno(Fpo)}}$, where $\mathbb{E}$ is the total electron energy and $E_{Fno(Fpo)}$ 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 $W_{n(p)}(\nu_{n(p)}, N^*, r_{d(a)})$.

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

A. Kane integration method (KIM)

In degenerate d(a)- GaSb 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 $x = -\mathbb{E}/\sqrt{W_{n(p)}} \equiv A_{n(p)} \times \nu_{n(p)} \times \exp\left(\frac{\mathcal{H}\times R_{sn(sp)}}{4\times\sqrt{|\nu_{n(p)}|}}\right)$,

and using an identity:

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

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:

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

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

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

noting that as a=1, $(it)^{-\frac{3}{2}} \times \exp\left\{-\frac{\left(t\sqrt{W_p}\right)^2}{2\hbar^2}\right\}$ 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: $\langle \mathbb{E}_k^{a-\frac{1}{2}} \rangle_{FPIM} \equiv \langle \mathbb{E}_k^{a-\frac{1}{2}} \rangle_{KIM}$, $\langle \mathbb{E}_k^{a-\frac{1}{2}} \rangle_{KIM}$ being determined in Eq. (13).

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

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

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

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

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

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

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

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

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

(ii) $\mathbb{E} \leq 0 -$ case.

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

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

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

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

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

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

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

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

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

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

C. Critical impurity density in the MIT

In degenerate d(a)- GaSb systems at T=0 K, in which $m_{n(p)}^*/m_o = m_{n(p)}/m_o = 0.047\ (0.3)$, as given in Section 2, using Eq. (13), for a=1, the density of states $\mathcal{D}(\mathbb{E})$ is defined by:

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

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

Here, E_{Fno} is determined in Eq. (A4) of the Appendix A, with $m_{n(p)}^*/m_o = m_{n(p)}/m_o$ and $\mathcal{H} = 0.1\ (0.1)$, respectively, being chosen such that the following determination of $N_{CDn(CDp)}^{EBT}(N, r_{d(a)})$ would be accurate.

Going back to the functions: H_n, K_n and F_n, given respectively in Equations (15-17), in which the factor $\frac{\langle \mathbb{E}_k^{\frac{1}{2}} \rangle_{KIM}}{f(a=1)}$ is now replaced by:

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

(19)

Therefore, $N_{CDn(CDp)}^{EBT}(N, r_{d(a)})$ can be defined by

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

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

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

where

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

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

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

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

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

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

Finally, Eq. (20) now yields:

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

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

The numerical results of $N_{CDn(CDp)}^{EBT}[N = N_{CDn(NDp)}(r_{d(a)})] \equiv N_{CDn(CDp)}^{EBT}(r_{d(a)})$, for a simplicity of presentation, evaluated using Eq. (21), are given in Table 2, confirming thus those of $N_{CDn(NDp)}(r_{d(a)})$, calculated using Eq. (3), with a precision of the order of 7.8% (5.9%), respectively. In other words, this critical d(a)-density $N_{CDn(NDp)}(r_{d(a))})$ can thus be explained by the density of electrons(holes) localized in the EBT, $N_{CDn(CDp)}^{EBT}(r_{d(a)})$.

So, the effective density of free electrons (holes), N^*, given in the parabolic conduction (valence) band of the degenerate d(a)- GaSb systems, can thus be expressed by:

$$N^* \equiv N - N_{CDn(NDp)} \cong N - N^{EBT}_{CDn(CDp)}. \quad (21b)$$

Then, as $N^* = N_{CDn(NDp)}$, according to the Fermi energy, $E_{Fno(Fpo)}(N^* = N_{CDn(NDp)}) \equiv \frac{\hbar^2 \times k^2_{Fn(Fp)}(N_{CDn(NDp)})}{2 \times m^*_{n(p)}}$, given in this parabolic conduction (valence) band (i.e. $\mathbb{E} \geq 0$), the value of the density of electrons(holes), $N^{EBT}_{CDn(CDp)}$, localized in the EBT ($\mathbb{E} \leq 0$), is almost equal to $N_{CDn(NDp)}$, as noted above. This can thus be expressed as:

$$N^{EBT}_{CDn(CDp)} \cong N_{CDn(NDp)}, \text{ as } N^* \equiv N_{CDn(NDp)}. \quad (21c)$$

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

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

where $\mathbb{E}_{Fn(Fp)}(N, T)$ 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:

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

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

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

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

where $C^{\beta}_p \equiv p(p-1)\ldots(p-\beta+1)/\beta!$ and the integral I_{β} is given by:

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

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

Then, some usual results of $G_{p\geq 1}(y)$ 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 $G_{p=1}(y \equiv \frac{\pi k_B T}{\mathbb{E}_{Fn(Fp)}} = \frac{\pi}{\xi_{n(p)}}) = 1$, 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 GaSb, as follows.

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

Here, $m^*_{n(p)}/m_o$ is chosen as: $m^*_{n(p)}/m_o = m_{Cn(Cp)}/m_o = 0.06(0.4)$, 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 $ohm^{-1} \times cm^{-1}$, the thermal conductivity by $\kappa(N^*, r_{d(a)}, T)$, expressed in $\frac{W}{cm\times K}$, and Lorenz number by $L = \frac{\pi^2}{3} \times \left(\frac{k_B}{q}\right)^2 = 2.4429637 \left(\frac{W\times ohm}{K^2}\right)$, 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:

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

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 $\underline{\mathbb{E} \geq 0}$, 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:

$$\sigma(N^*, r_{d(a)}, T) \equiv \left[\frac{q^2 \times k_{Fn(Fp)}}{\pi \times \hbar} \times \frac{k_{Fn(Fp)}}{k_{sn(sp)}(N^*)} \times \left[k_{Fn(Fp)} \times a_{Bn(Bp)}(r_{d(a)})\right] \times \left(\frac{\mathbb{E}_{Fno(Fpo)}(N^*, T=0)}{\eta_{n(p)}(N^*, r_{d(a)})}\right)^{1/2}\right] \times [G_2(N^*, T) \times \left(\frac{\mathbb{E}_{Fn(Fp)}(N^*, T)}{\mathbb{E}_{Fno(Fpo)}(N^*, T=0)}\right)^2], \; k_{Fn(Fp)}(N^*) \equiv \left(3\pi^2 N^*/g_{c(v)}\right)^{1/3}, \quad (27)$$

which also determine the resistivity as: $\rho(N^*, r_{d(a)}, T) \equiv 1/\sigma(N^*, r_{d(a)}, T)$, noting that $N^* \equiv N - N_{CDn(NDp)}(r_{d(a)})$. 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 K, as noted in Eq. (22), $\sigma(N^*, r_{d(a)}, T = 0K)$ is proportional to $\mathbb{E}_{Fno(Fpo)}^2$, or to $(N^*)^{4/3}$. Thus, $\sigma(N^* = 0, r_{d(a)}, T = 0K) = 0$ at $N^* = 0$, at which the metal-insulator transition (MIT) occurs.

A. Electrical properties

The relaxation time τ is related to σ by:

$\tau(N^*, r_{d(a)}, T) \equiv \sigma(N^*, r_{d(a)}, T) \times \frac{m_{Cn(Cp)}}{q^2 \times N^*}$. Therefore, the mobility μ 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= 0K, $\mu(N^*, r_{d(a)}, T = 0K)$ is thus proportional to $(N^*)^{1/3}$, since $\sigma(N^*, r_{d(a)}, T = 0K)$ is proportional to $(N^*)^{4/3}$. Thus, $\mu(N^* = 0, r_{d(a)}, T = 0K) = 0$ at $N^* = 0$, at which the metal-insulator transition (MIT) occurs.

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

$r_H(N^*, T) \equiv \frac{\langle \tau^2 \rangle_{FDDF}}{[\langle \tau \rangle_{FDDF}]^2} = \frac{G_4(y)}{[G_2(y)]^2}$, 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=0K, since $r_H(N^*, T = 0K) = 1$, one gets:

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

Further, as discussed in Eq. (21c) and at $T = 0K$, we can also determine the values of these electrical-and-thermoelectric coefficients, localized in the EBT for $\mathbb{E} \leq 0$, by replacing: $N^* = N_{CDn(NDp)} \cong N_{CDn(CDp)}^{EBT}$ into Equations (27, 28, 29), and Eq. (A7) of the Appendix A, for $\mathbb{E} \geq 0$, to obtain: $\sigma^{EBT}(N^* = N_{CDn(NDp)}, r_{d(a)})$, $\mu^{EBT}(N^* = N_{CDn(NDp)}, r_{d(a)})$, $\mu_H^{EBT}(N^* = N_{CDn(NDp)}, r_{d(a)})$ and $D^{EBT}(r_{d(a)})$. Those numerical results are reported in following Table 5.

Table 5. Here, the values of the electrical-and-thermoelectric coefficients, obtained in the exponential tails (i.e. $\mathbb{E} \leq 0$), as: $\sigma^{EBT}(r_{d(a)})$, $\mu^{EBT}(r_{d(a)})$, $\mu_H^{EBT}(r_{d(a)})$ and $D^{EBT}(r_{d(a)})$ are reported, and their variations with increasing $r_{d(a)}$ are represented by the arrows: ↗ and ↘.

d- GaSb systems		P	As	Te	Sb	Sn
r_d (nm) [4]	↗	0.110	0.118	0.132	0.136	0.140
$\sigma^{EBT}(r_d)$ in $\frac{10^4}{ohm\times cm}$	↗	3.774	4.152	4.475	4.492	4.509
$\mu^{EBT}(r_d)$ in $\frac{10^5\times cm^2}{V\times s}$	↘	5.024	4.117	3.531	3.504	3.477
$\mu_H^{EBT}(r_d)$ in $\frac{10^5\times cm^2}{V\times s}$	↘	5.024	4.117	3.531	3.504	3.477
$D^{EBT}(r_d)$ in $\frac{10^4\times cm^2}{s}$	↘	1.228	1.225	1.2232	1.2231	1.2230

a- GaSb systems		Ga(Al, Mn)	Mg	In
r_a (nm) [4]	↗	0.126	0.140	0.144
$\sigma^{EBT}(r_a)$ in $\frac{10^3}{ohm\times cm}$	↗	1.234	1.272	1.300
$\mu^{EBT}(r_a)$ in $\frac{10^3\times cm^2}{V\times s}$	↘	9.627	8.399	7.741
$\mu_H^{EBT}(r_a)$ in $\frac{10^3\times cm^2}{V\times s}$	↘	9.627	8.399	7.741
$D^{EBT}(r_a)$ in $\frac{10\times cm^2}{s}$	↘	5.041	4.915	4.853

Furthermore, in the degenerate d(a)-GaSb systems, at T=4.2 K and T=77 K, the numerical results of σ, μ, μ_H, and the diffusion coefficient D, evaluated respectively by using Equations (27, 28, 29, A8 of the Appendix A), are reported in following Table 6.

Table 6. Here, one notes 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: $\sigma(N^*)$, $D(N^*)$, $\mu(N^*)$ and $\mu_H(N^*)$ increase, with increasing N.

Donor	P	As	Te	Sb	Sn
r_d (nm) [4] ↗	0.110	0.118	0.132	0.136	0.140
In the following, our numerical results of (σ, μ, μ_H, D) at 4.2K, expressed respectively in $\left(\frac{10^5}{ohm\times cm}, \frac{10^5\times cm^2}{V\times s}, \frac{10^5\times cm^2}{V\times s}, \frac{10^5\times cm^2}{s}\right)$					
$N(10^{18}\ cm^{-3})$					
3	2.23, 5.50, 5.50, 0.41	1.68, 4.41, 4.42, 0.32	1.32, 3.72, 3.72, 0.25	1.30, 3.69, 3.69, 0.25	1.28, 3.66, 3.66, 0.25
10	9.20, 6.03, 6.03, 1.10	7.27, 4.84, 4.84, 0.87	6.03, 4.09, 4.09, 0.73	5.97, 4.05, 4.05, 0.72	5.91, 4.02, 4.02, 0.71
40	42.5, 6.71, 6.71, 3.16	34.0, 5.39, 5.39, 2.53	28.6, 4.55, 4.55, 2.13	28.3, 4.51, 4.51, 2.10	28.1, 4.47, 4.47, 2.09
70	78.2, 7.02, 7.02, 4.81	62.6, 5.63, 5.63, 3.85	52.7, 4.75, 4.75, 3.24	52.2, 4.71, 4.71, 3.22	51.8, 4.67, 4.67, 3.19

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

N(10^{18} cm^{-3})					
3	2.25, 5.56, 5.81, 0.42	1.70, 4.47, 4.69, 0.32	1.33, 3.77, 3.97, 0.26	1.32, 3.74, 3.94, 0.26	1.30, 3.71, 3.91, 0.25
10	9.22, 6.04, 6.08, 1.10	7.28, 4.85, 4.89, 0.87	6.04, 4.09, 4.13, 0.73	5.98, 4.06, 4.09, 0.72	5.92, 4.02, 4.06, 0.72
40	42.5, 6.72, 6.72, 3.16	34.0, 5.39, 5.40, 2.53	28.6, 4.55, 4.55, 2.13	28.3, 4.51, 4.51, 2.11	28.1, 4.47, 4.47, 2.09
70	78.2, 7.02, 7.03, 4.81	62.6, 5.63, 5.64, 3.85	52.7, 4.75, 4.76, 3.25	52.2, 4.71, 4.71, 3.22	51.8, 4.67, 4.67, 3.19

Acceptor		Ga(Al, Mn)	Mg	In
r_a (nm) [4]	↗	0.126	0.140	0.144

In the following, our numerical results of (σ, μ, μ_H, D) at 4.2K, expressed respectively in $\left(\frac{10^4}{\text{ohm}\times\text{cm}}, \frac{10^3\times \text{cm}^2}{\text{V}\times\text{s}}, \frac{10^3\times \text{cm}^2}{\text{V}\times\text{s}}, \frac{10^2\times\text{cm}^2}{\text{s}}\right)$

N(10^{19} cm^{-3})			
3	0.29, 8.19, 8.25, 0.84	0.24, 7.45, 7.51, 0.73	0.22, 7.04, 7.09, 0.67
10	1.11, 7.51, 7.52, 2.00	0.98, 6.76, 6.77, 1.78	0.91, 6.33, 6.34, 1.66
40	4.67, 7.44, 7.44, 5.21	4.15, 6.64, 6.64, 4.64	3.86, 6.19, 6.19, 4.32
70	8.34, 7.52, 7.52, 7.70	7.41, 6.70, 6.70, 6.85	6.89, 6.24, 6.24, 6.37

In the following, our numerical results of (σ, μ, μ_H, D) at **77**K, expressed respectively in $\left(\frac{10^4}{\text{ohm}\times\text{cm}}, \frac{10^3\times \text{cm}^2}{\text{V}\times\text{s}}, \frac{10^3\times \text{cm}^2}{\text{V}\times\text{s}}, \frac{10^2\times\text{cm}^2}{\text{s}}\right)$

N(10^{19} cm^{-3})			
3	0.53, 15.2, 40.7, 1.56	0.49, 14.8, 41.5, 1.44	0.46, 14.8, 43.0, 1.37
10	1.20, 8.14, 10.6, 2.31	1.06, 7.34, 9.63, 2.06	0.98, 6.88, 9.06, 1.92
40	4.73, 7.53, 7.92, 5.32	4.20, 6.73, 7.07, 4.74	3.91, 6.27, 6.60, 4.42
70	8.39, 7.56, 7.75, 7.78	7.46, 6.74, 6.91, 6.92	6.93, 6.28, 6.43, 6.44

Acceptor	Ga(Al)	Mg	In

In the following, our numerical results of (σ, μ, μ_H, D) at 4.2K, expressed respectively in $\left(\frac{10^4}{\text{ohm}\times\text{cm}}, \frac{10^3\times \text{cm}^2}{\text{V}\times\text{s}}, \frac{10^3\times \text{cm}^2}{\text{V}\times\text{s}}, \frac{10^2\times\text{cm}^2}{\text{s}}\right)$

N(10^{19} cm^{-3})			
3	0.29, 8.19, 8.25, 0.84	0.24, 7.45, 7.51, 0.73	0.22, 7.04, 7.09, 0.67
10	1.11, 7.51, 7.52, 2.00	0.98, 6.76, 6.77, 1.78	0.91, 6.33, 6.34, 1.66
40	4.67, 7.44, 7.44, 5.21	4.15, 6.64, 6.64, 4.64	3.86, 6.19, 6.19, 4.32
70	8.34, 7.52, 7.52, 7.70	7.41, 6.70, 6.70, 6.85	6.89, 6.24, 6.24, 6.37

In the following, our numerical results of (σ, μ, μ_H, D) at **77**K, expressed respectively in $\left(\frac{10^4}{\text{ohm}\times\text{cm}}, \frac{10^3\times \text{cm}^2}{\text{V}\times\text{s}}, \frac{10^3\times \text{cm}^2}{\text{V}\times\text{s}}, \frac{10^2\times\text{cm}^2}{\text{s}}\right)$

N(10^{19} cm^{-3})			
3	0.53, 15.2, 40.7, 1.56	0.49, 14.8, 41.5, 1.44	0.46, 14.8, 43.0, 1.37
10	1.20, 8.14, 10.6, 2.31	1.06, 7.34, 9.63, 2.06	0.98, 6.88, 9.06, 1.92
40	4.73, 7.53, 7.92, 5.32	4.20, 6.73, 7.07, 4.74	3.91, 6.27, 6.60, 4.42
70	8.39, 7.56, 7.75, 7.78	7.46, 6.74, 6.91, 6.92	6.93, 6.28, 6.43, 6.44

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, is given in the n(p)-type degenerate GaSb crystals, as:

$$S(N^*, T) \equiv (\mp)\frac{\pi^2}{3} \times \frac{k_B}{q} \times k_B T \times \frac{\partial \ln\sigma(\mathbb{E})}{\partial \mathbb{E}}\Big]_{\mathbb{E}=\mathbb{E}_{Fn(Fp)}}.$$

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

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

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

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

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

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

$$Pt(N^*, T) \equiv T \times S(N^*, T). \quad (32)$$

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

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

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

Then, being inspired from this $L_{Kim}(\lfloor S \rfloor)$-expression, we also propose another one, given in the n(p)-type degenerate GaSb, as:

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

where $\left|RD_{L,L_{VC}}\right|$ 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)-GaSb, defined by physical conditions : $N = 10^{20} cm^{-3}$ and T (=3K 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 $\left|RD_{\kappa,\kappa_{App.}}\right|_T$ by Eq. (25b), $S(N^*, T)$, $Ts(N^*, T)$, $Pt(N^*, T)$ and $ZT(N^*, T)$ by Equations (30, 31, 32, 33) respectively, and finally, $\left|RD_{L,L_{VC}}\right|$ 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 $r_{d(a)}$, due to the impurity size effect, $N_{CDn}(r_d)$, increases, since N(=10^{20} cm^{-3}) is very high, N^* therefore decreases slowly, explaining the slow decrease (↘) in $\frac{\mathbb{E}_{Fn(Fp)}(N^*,T=300K)}{k_BT}$, σ, κ, C_κ, and $\kappa_{App.}$, (ii) the numerical result: $\left|RD_{\kappa,\kappa_{App.}}\right|_{300K} = 0.129\%$ (confirms the $\kappa_{App.}$-law, as given in Eq. (25b), and finally, (iii) $\left|RD_{L,L_{VC}}\right| = 1.534\times 10^{-6}$ thus confirms in the degenerate GaSb -case the well-known Wiedemann-Frank, given in Eq. (25a), is found to be exact.

Donor	P	**As**	Te	Sb	Sn
Highly degenerate d-GaSb systems for N=10^{20} cm^{-3} and at T=3K and T=300K, noting that $N^* \equiv N - N_{CDn}(r_d)$					
$\frac{E_{Fn}(N^*,T=300K)}{k_BT} \gg 1$	50.50	50.40	50.39	50.38	50.38
$\sigma_{(T=3K)}$ $\left(\frac{10^7}{ohm\times cm}\right)$ ↘	1.1524	0.9232	0.7772	0.7705	0.7636
$\sigma_{(T=300K)}$ $\left(\frac{10^7}{ohm\times cm}\right)$ ↘	1.1540	0.9243	0.7782	0.7715	0.7646
$\kappa_{(T=3K)}$ $\left(\frac{W}{cm\times K}\right)$ ↘	0.8446	0.6766	0.5696	0.5647	0.5597
$\kappa_{(T=300K)}$ $\left(\frac{W}{cm\times K}\right)$ ↘	84.567	67.745	57.040	56.542	56.040
C_κ $\left(\frac{W}{cm\times K^2}\right)$ ↘	0.2815	0.2255	0.1899	0.1882	0.1865
$\kappa_{App.}(300K)$ $\left(\frac{W}{cm\times K}\right)$ ↘	84.458	67.657	56.963	56.469	55.968
$\left\|RD_{\kappa,\kappa_{App.}}\right\|_{300K}$ in %	0.129	0.129	0.129	0.129	0.129
$S_{(T=3K)}$ $\left(\frac{10^{-7}\times V}{K}\right)$.	−1.123	−1.124	−1.126	−1.126	−1.126
$S_{(T=300K)}$ $\left(\frac{10^{-5}\times V}{K}\right)$	−1.121	−1.122	−1.124	−1.124	−1.124
$Ts_{(T=3K)}$ $\left(\frac{10^{-7}\times V}{K}\right)$	−1.123	−1.124	−1.126	−1.126	−1.126
$Ts_{(T=300K)}$ $\left(\frac{10^{-5}\times V}{K}\right)$	−1.117	−1.118	−1.120	−1.120	−1.120
$Pt_{(T=3K)}$ $(10^{-7}\times V)$	−3.370	−3.374	−3.377	−3.377	−3.378
$Pt_{(T=300K)}$ $(10^{-3}\times V)$	−3.364	−3.368	−3.371	−3.371	−3.372
$ZT_{(T=3K)}$ $(\times 10^{-7})$	5.165	5.177	5.188	5.188	5.189
$ZT_{(T=300K)}(\times 10^{-3})$	5.147	5.158	5.169	5.170	5.171
$\left\|RD_{L,L_{VC}}\right\|$ in 10^{-6} at 3 K	1.534	1.534	1.534	1.534	1.534
$\|RD\|$ in 10^{-6} at 300K	1.535	1.535	1.5345	1.535	1.535

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^{20} cm^{-3}) is very high, N^* therefore decreases slowly, explaining the slow decrease (↘) in $\frac{\mathbb{E}_{Fp}(N^*,T=300K)}{k_BT}$, σ, κ, C_κ, and $\kappa_{App.}$, (ii) the numerical result: $\left|RD_{\kappa,\kappa_{App.}}\right|_{300K} \simeq 5.24\%$ confirms the $\kappa_{App.}$-law, as given in Eq. (25b), and finally, (iii) $\left|RD_{L,L_{VC}}\right| \simeq 1.535\times 10^{-6}$ thus confirms in the degenerate GaSb-case the well-known Wiedemann-Frank, given in Eq. (25a), is found to be exact.

Acceptor	Ga (Al)	Mg	In
Highly degenerate a- GaSb systems for N=10^{20} cm^{-3} and T=3K and T=300K			
$\frac{\mathbb{E}_{Fp}(N^*,T=300K)}{k_BT} \gg 1$ ↘	7.72	7.71	7.71
$\sigma_{(T=3K)}$ $\left(\frac{10^5}{ohm\times cm}\right)$ ↘	1.21	1.07	1.00

$\sigma_{(T=300K)}\left(\frac{10^5}{ohm\times cm}\right)$ ↘	1.27	1.13	1.05
$\kappa_{(T=3K)}\left(\frac{10^{-3}\times W}{cm\times K}\right)$ ↘	8.8514	7.8674	7.3129
$\kappa_{(T=300K)}\left(\frac{W}{cm\times K}\right)$ ↘	0.9339	0.8302	0.7717
$C_\kappa\left(\frac{10^{-3}\times W}{cm\times K^2}\right)$ at T=3K ↘	2.9505	2.6225	2.4376
$\kappa_{App.}(300K)\left(\frac{W}{cm\times K}\right)$ ↘	0.8851	0.7867	0.7313
$\left\|RD_{\kappa,\kappa_{App.}}\right\|_{300K}$ in %	5.23	5.23	5.24
$Sb_{(T=3K)}\left(\frac{10^{-7}\times V}{K}\right)$	-7.506	-7.513	-7.518
$Sb_{(T=300K)}\left(\frac{10^{-5}\times V}{K}\right)$	-6.958	-6.963	-6.968
$Ts_{(T=3K)}\left(\frac{10^{-7}\times V}{K}\right)$	-7.505	-7.513	-7.518
$Ts_{(T=300K)}\left(\frac{10^{-5}\times V}{K}\right)$	-5.953	-5.956	-5.958
$Pt_{(T=3K)}\ (10^{-6}\times V)$	-2.252	-2.254	-2.255
$Pt_{(T=300K)}\ (10^{-2}\times V)$	-2.087	-2.089	-2.090
$ZT_{(T=3K)}\ (\times 10^{-5})$	2.306	2.310	2.314
$ZT_{(T=300K)}$	0.198	0.198	0.199
$\left\|RD_{L,L_{VC}}\right\|$ in 10^{-6} at 3 K	1.534	1.534	1.534
$\left\|RD_{L,L_{VC}}\right\|$ in 10^{-6} at 300 K	1.537	1.537	1.537

Secondly, in the degenerate d(a)-GaSb, 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: $S(N^*,T)$ by Eq. (30), $\left|RD_{L,L_{VC}}\right|$ 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 9-10.

Table 9. Here, for a given N^* and for a given degenerate d-GaSb system, with increasing T, the reduced Fermi-energy ξ_n decreases, and other thermoelectric coefficients are in variations, as indicated by the arrows as: (↗, ↘). One notes that with increasing T: (i) for $\xi_n = 1.814$, while the numerical results of S present a same minimum $(S)_{min.}\left(=-1.563\times 10^{-4}\frac{V}{K}\right)$, those of ZT show a same maximum $ZT_{max.}(=\mathbf{1})$, (ii) for $\xi_n = 1$, S and ZT present same results: $-1.322\times 10^{-4}\frac{V}{K}$ and 0.715, respectively, (iii) for $\xi_n =$ 1.814 and $\xi_n = 1$, $(ZT)_{Mott} = \frac{\pi^2}{3\times\xi_n^2}$ present same results: $\simeq 1$ and 3.290, respectively, and finally, (iv) the maximal value of $\left|RD_{L,L_{VC}}\right|$ is approximated to 1.541×10^{-6}, suggesting that in the degenerate GaSb -case the Wiedemann-Frank, given in Eq. (25a), is exact.

In the degenerate P- GaSb system, $N^* \equiv N - N_{CDn}(r_P) \equiv N_{CDn}(r_P)$; $N = 1.1\times N_{CDn}(r_P) = 5.157\times 10^{17}\ cm^{-3}$

T(K) ↗	5		10		**41.32**		45		**56.228547**		56.5
ξ_n ↘	18.40		9.305		**1.814**		1.557		**1**		0.989
$S\left(10^{-4}\frac{V}{K}\right)$	-0.305	↘	-0.587	↘	$\mathbf{-1.563}$	↗	-1.546	↗	$\mathbf{-1.322}$	↗	-1.314
$\left\|RD_{L,L_{VC}}\right\|$ in 10^{-6}	1.536		1.537		1.541		1.541		1.540		1.540
ZT	0.038	↗	0.141	↗	**1**	↘	0.979	↘	**0.715**	↘	0.706
$(ZT)_{Mott} = \frac{\pi^2}{3\times\xi_n^2}$ ↗	0.010		0.038		**0.9999**		1.340		3.290		3.365
$T_s\left(10^{-4}\frac{V}{K}\right)$	-0.297	↘	-0.527	↗	-1.44×10^{-4}	↗	0.399	↗	1.657	↗	1.686
Pt $(10^{-3}V)$	-0.152	↘	-0.587	↘	-6.458	↘	-6.959	↘	-7.432	↗	-7.422

In the degenerate As- GaSb system, $N^* \equiv N - N_{CDn}(r_{As}) \equiv N_{CDn}(r_{As})$; $N = 1.1\times N_{CDn}(r_{As}) = 6.924\times 10^{17} cm^{-3}$

T(K) ↗	5		10	**50.29**	55	**68.433628**	68.5

ξ_n	↘	22.37		11.27		**1.814**		1.555		**1**	0.998
S $\left(10^{-4}\frac{V}{K}\right)$		−0.252	↘	−0.490	↘	**−1.563**	↗	−1.545	↗	**−1.322**	↗ −1.320
$\left\|RD_{L,L_{VC}}\right\|$ in 10^{-6}		1.535		1.536		1.541		1.541		1.540	1.540
ZT		0.026	↗	0.098	↗	**1**	↘	0.977	↘	**0.715**	↘ 0.713
$(ZT)_{Mott}=\frac{\pi^2}{3\times\xi_n^2}$	↗	0.006		0.026		**0.9999**		1.361		3.290	3.305
Ts $\left(10^{-4}\frac{V}{K}\right)$		−0.025	↘	−0.456	↗	-5.77×10^{-5}	↗	0.420	↗	1.657	↗ 1.663
Pt $(10^{-3}V)$		− 0.126	↘	−0.490	↘	−7.860	↘	−8.495	↘	−9.045	↗ −9.043

In the degenerate Te- GaSb system, $N^* \equiv N - N_{CDn}(r_{Te}) \equiv N_{CDn}(r_{Te})$; $N = 1.1 \times N_{CDn}(r_{Te}) = 8.699 \times 10^{17} cm^{-3}$

T(K)	↗	5		10		**58.55**		65		**79.6784292**	80
ξ_n	↘	26.03		13.09		**1.814**		1.514		**1**	0.990
S $\left(10^{-4}\frac{V}{K}\right)$		−0.217	↘	−0.425	↘	**−1.563**	↗	−1.538	↗	**−1.322**	↗ −1.315
$\left\|RD_{L,L_{VC}}\right\|$ in 10^{-6}		1.535		1.536		1.541		1.541		1.540	1.540
ZT		0.019	↗	0.074	↗	**1**	↘	0.968	↘	**0.715**	↘ 0.708
$(ZT)_{Mott}=\frac{\pi^2}{3\times\xi_n^2}$	↗	0.005		0.019		**0.9997**		1.435		3.290	3.353
Ts $\left(10^{-4}\frac{V}{K}\right)$		−0.214	↘	−0.403	↗	-3.17×10^{-4}	↗	0.496	↗	1.657	↗ 1.682
Pt $(10^{-3}V)$		− 0.108	↘	−0.425	↘	−9.151	↘	−9.996	↘	−10.531	↗ −10.520

In the degenerate Sb- GaSb system, $N^* \equiv N - N_{CDn}(r_{Sb}) \equiv N_{CDn}(r_{Sb})$; $N = 1.1 \times N_{CDn}(r_{Sb}) = 8.8 \times 10^{17} cm^{-3}$

T(K)	↗	5		10		**59**		65		**80.29159**	80.5
ξ_n	↘	26.23		13.18		**1.814**		1.535		**1**	0.994
S $\left(10^{-4}\frac{V}{K}\right)$		−0.215	↘	−0.422	↘	**−1.563**	↗	−1.541	↗	**−1.322**	↗ −1.317
$\left\|RD_{L,L_{VC}}\right\|$ in 10^{-6}		1.535		1.536		1.541		1.541		1.540	1.540
ZT		0.019	↗	0.073	↗	**1**	↘	0.973	↘	**0.715**	↘ 0.710
$(ZT)_{Mott}=\frac{\pi^2}{3\times\xi_n^2}$	↗	0.005		0.019		**0.9997**		1.396		3.290	3.330
Ts $\left(10^{-4}\frac{V}{K}\right)$		−0.212	↘	−0.400	↗	-3.59×10^{-4}	↗	0.457	↗	1.657	↗ 1.673
Pt $(10^{-3}V)$		− 0.107	↘	−0.422	↘	−9.222	↘	−10.019	↘	−10.612	↗ −10.605

In the degenerate Sn- GaSb system, $N^* \equiv N - N_{CDn}(r_{Sn}) \equiv N_{CDn}(r_{Sn})$; $N = 1.1 \times N_{CDn}(r_{Sn}) = 8.905 \times 10^{17} cm^{-3}$

T(K)	↗	5		10		**59.47**		65		**80.92887**	81
ξ_n	↘	26.43		13.29		**1.814**		1.557		**1**	0.998
S $\left(10^{-4}\frac{V}{K}\right)$		−0.213	↘	−0.419	↘	**−1.563**	↗	−1.545	↗	**−1.322**	↗ −1.320
$\left\|RD_{L,L_{VC}}\right\|$ in 10^{-6}		1.535		1.536		1.541		1.541		1.540	1.540
ZT		0.019	↗	0.072	↗	**1**	↘	0.978	↘	**0.715**	↘ 0.713
$(ZT)_{Mott}=\frac{\pi^2}{3\times\xi_n^2}$	↗	0.005		0.019		**0.9998**		1.357		3.290	3.303
Ts $\left(10^{-4}\frac{V}{K}\right)$		−0.211	↘	−0.398	↗	-2.34×10^{-4}	↗	0.417	↗	1.657	↗ 1.663
Pt $(10^{-3}V)$		− 0.107	↘	−0.419	↘	−9.295	↘	−10.042	↘	−10.696	↗ −10.694

Table 10. Here, for a given N^* and for a given degenerate a- GaSb 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 $\xi_p = 1.814$, S and ZT present same results: $-1.322 \times 10^{-4}\frac{V}{K}$ and 0.715, 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 $\xi_p = 1.814$ and $\xi_p = 1$, $(ZT)_{Mott} = \frac{\pi^2}{3\times\xi_p^2}$ present same results: $\simeq 1$ and 3.290, respectively, and finally, (iv) the maximal value of $\left|RD_{L,L_{VC}}\right|$ is approximated to 1.541×10^{-6}, suggesting that in the degenerate GaSb -case the Wiedemann-Frank, given in Eq. (25a), is exact.

In the degenerate Ga- GaSb system, $N^* \equiv N - N_{CDn}(r_{Ga}) \equiv N_{CDn}(r_{Ga})$; $N = 2 \times N_{CDn}(r_{Ga}) = 1.6 \times 10^{18}\ cm^{-3}$

T(K)	↗	5		10		**41.078**		45		**55.902081**	56
ξ_p	↘	18.29		9.25		**1.814**		1.550		**1**	0.996
S $\left(10^{-4}\frac{V}{K}\right)$		−0.307	↘	−0.590	↘	**−1.563**	↗	−1.544	↗	**−1.322**	↗ −1.319

$\left\|RD_{L,L_{VC}}\right\|$ in 10^{-6}	1.536		1.537		1.541		1.541		1.540		1.540
ZT	0.038	↗	0.142	↗	**1**	↘	0.976	↘	**0.715**	↘	0.712
$(ZT)_{Mott}=\frac{\pi^2}{3\times\xi_n^2}$	↗ 0.010		0.038		**0.9997**		1.368		3.290		3.317
Ts $\left(10^{-4}\frac{V}{K}\right)$	−0.299	↘	−0.530	↗	-3.66×10^{-4}	↗	0.428	↗	1.657	↗	1.668
Pt $(10^{-3}V)$	− 0.153	↘	−0.590	↘	−6.420	↘	−6.948	↘	−7.388	↗	−7.385

In the degenerate Mg- GaSb system, $N^* \equiv N - N_{CDn}(r_{Mg}) \equiv N_{CDn}(r_{Mg})$; $N = 2\times N_{CDn}(r_{Mg}) = 1.89\times10^{18}\ cm^{-3}$

T(K)	↗	5		10		**45.91**		50		**62.47071**		62.5
ξ_p	↘	20.4		10.3		**1.814**		1.566		**1**		0.999
S $\left(10^{-4}\frac{V}{K}\right)$		−0.275	↘	−0.533	↘	**−1.563**	↗	−1.546	↗	**−1.322**	↗	−1.321
$\left\|RD_{L,L_{VC}}\right\|$ in 10^{-6}		1.535		1.537		1.541		1.541		1.540		1.540
ZT		0.031	↗	0.116	↗	**1**	↘	0.979	↘	**0.715**	↘	0.714
$(ZT)_{Mott}=\frac{\pi^2}{3\times\xi_n^2}$	↗	0.008		0.031		**1.0001**		1.341		3.290		3.297
Ts $\left(10^{-4}\frac{V}{K}\right)$		−0.269	↘	−0.489	↗	1.30×10^{-4}	↗	0.399	↗	1.657	↗	1.660
Pt $(10^{-3}V)$		− 0.138	↘	−0.533	↘	−7.176	↘	−7.732	↘	−8.257	↗	−8.256

In the degenerate In- GaSb system, $N^* \equiv N - N_{CDn}(r_{In}) \equiv N_{CDn}(r_{In})$; $N = 2\times N_{CDn}(r_{In}) = 2.096\times10^{18}\ cm^{-3}$

T(K)	↗	5		10		**49.184**		50		**66.935987**		67
ξ_p	↘	21.9		11.03		**1.814**		1.765		**1**		0.998
S $\left(10^{-4}\frac{V}{K}\right)$		−0.257	↘	−0.501	↘	**−1.563**	↗	−1.562	↗	**−1.322**	↗	−1.320
$\left\|RD_{L,L_{VC}}\right\|$ in 10^{-6}		1.535		1.537		1.541		1.541		1.540		1.540
ZT		0.027	↗	0.102	↗	**1**	↘	0.9992	↘	**0.715**	↘	0.713
$(ZT)_{Mott}=\frac{\pi^2}{3\times\xi_n^2}$	↗	0.007		0.027		**0.9996**		1.056		3.290		3.305
Ts $\left(10^{-4}\frac{V}{K}\right)$		−0.252	↘	−0.464	↗	-5.37×10^{-4}	↗	0.072	↗	1.657	↗	1.663
Pt $(10^{-3}V)$		− 0.129	↘	−0.501	↘	−7.687	↘	−7.812	↘	−8.847	↗	−8.845

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 $\left|RD_{L,L_{VC}}\right|$ is found to be 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, $\xi_{n(p)} \simeq 1$. In other word, our above $L_{VC}\left(N^*, T, r_{d(a)}\right)$-expression, given in Eq. (25b), is not useful in the present n(p)-type degenerate GaSb crystals.

6. Concluding remarks

In the n(p)-type degenerate GaSb-crystals, 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, $\varepsilon(r_{d(a)})$, 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, $\mathbb{E}_{Fn(Fp)}(N^*, T)$, 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, $Sb(N^*, T)$, 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 some new consequences are given as follows.

(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,

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

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

(c) As given in Eq. (27), the electrical conductivity, $\sigma(N^*, r_{d(a)}, T)$, is proportional to $\mathbb{E}^2_{Fno(Fpo)}$ or to $(N^*)^{4/3}$, giving rise to: $\sigma(N^* = 0, r_{d(a)}, T = 0) = 0$, and therefore, as discussed in Equations (27, 28, 29), and Eq. (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 $D(N^* = 0, r_{d(a)}, T = 0K) = 0$, being new results.

(d) In Table 5, the values of these electrical-and-thermoelectric coefficients, localized in the EBT for $\mathbb{E} \leq 0$, determined by replacing: $N^* = N_{CDn(NDp)} \cong N^{EBT}_{CDn(CDp)}$ into Equations (27, 28, 29), and Eq. (A7) of the Appendix A, for $\mathbb{E} \geq 0$, are reported.

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 $N^{EBT}_{CDn(CDp)}(r_{d(a)})$ are found to be equal to: 7.8% (5.9%), 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, $N^{EBT}_{CDn(CDp)}(r_{d(a)})$.

(2) In Table 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: $\sigma(N^*)$, $D(N^*)$, $\mu(N^*)$ and $\mu_H(N^*)$ increase, 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 $N(= 10^{20}\ cm^{-3})$ is very high, N^* therefore decreases very slowly, explaining the slow decrease (↘) in $\frac{E_{Fn(Fp)}(N^*,T=300K)}{k_BT}$, σ, κ, C_κ, and $\kappa_{App.}$, (ii) the numerical results:

$\left|RD_{\kappa,\kappa_{App.}}\right|_{300K} \simeq 0.13\ \%\ (5.24\ \%)$, respectively, confirm the $\kappa_{App.}$-law, as that given in Eq. (25b), and finally, (iii) $\left|RD_{L,L_{VC}}\right| \simeq 1.54 \times 10^{-6}$ thus confirms that in the degenerate GaSb-case the well-known Wiedemann-Frank law, given in Eq. (25a), is found to be exact.

(4) In Tables 9-10, for a given $N = 1.1\ (2) \times N_{CDn(NDp)}(r_{d(a)})$, and for a given degenerate d(a)-GaSb system, with increasing T, the reduced Fermi-energy $\xi_{n(p)}$ decreases, and other thermoelectric coefficients are in variations, as indicated by the arrows: (↗, ↘). One notes here that with increasing T: **(i)** for $\xi_{n(p)} = 1.814$, while the values of S present a same minimum $(S)_{min.}\left(=-1.563 \times 10^{-4}\frac{V}{K}\right)$, those of ZT show a same maximum $ZT_{max.}(=\mathbf{1})$, **(ii)** for $\xi_n = 1$, those of S and those of ZT present same results: S($=-1.322 \times 10^{-4}\frac{V}{K}$) and ZT (=0.715), respectively, **(iii)** for $\xi_{n(p)} = 1.814$ 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}, confirming that in the degenerate GaSb-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 here.

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 GaSb-crystals, the Fermi energy $E_{Fn(Fp)} \equiv [E - E_c](E_{Fp} \equiv [E_v - E_{fp}])$, $E_{c(v)}$ 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:

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

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 GaSb is determined by :

$$\frac{\mathbb{E}_{Fn(Fp)}(u)}{k_B T} = \frac{G(u)+Au^B F(u)}{1+Au^B} = \xi_{n(p)}(u) \equiv \frac{V(u)}{W(u)},\ A = 0.0005372 \text{ and } B = 4.82842262, \qquad (A2)$$

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 $G(u) \simeq Ln(u) + 2^{-\frac{3}{2}} \times u \times e^{-du}$ 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:

$$\mathbb{E}_{Fn(Fp)}\left(N^*, r_{d(a)}, T\right) \equiv \mathbb{E}_{Fn(Fp)}(N^*, T) = \mathbb{E}_{Fno(Fpo)}(u) \times \left(1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}}\right)^{-\frac{2}{3}}. \quad (A3)$$

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

$$\mathbb{E}_{Fno(Fpo)}(N^*) \equiv \frac{\hbar^2 \times k^2_{Fn(Fp)}(N^*)}{2 \times m^*_{n(p)}}, \quad (A4)$$

being proportional to $(N^*)^{2/3}$, and equal to 0, $\mathbb{E}_{Fno(Fpo)}(N^* = 0) = 0$, according to the MIT, as discussed in Section 2 and 3.

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

$$\frac{D\left(N^*, r_{d(a)}, T\right)}{\mu\left(N^*, r_{d(a)}, T\right)} \equiv \frac{N}{q} \times \frac{d\mathbb{E}_{Fn(Fp)}}{dN} \equiv \frac{k_B \times T}{q} \times \left(u \frac{d\theta_{n(p)}}{du}\right), \quad (A.5)$$

where $D\left(N^*, r_{d(a)}, T\right)$ is the diffusion coefficient, $\theta_n(u)$ is defined in (A2), and the mobility $\mu\left(N^*, r_{d(a)}, T\right)$ 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,

$$\frac{D\left(N^*, r_{d(a)}, T\right)}{\mu\left(N^*, r_{d(a)}, T\right)} = \frac{k_B \times T}{q} \times u \frac{V'(u) \times W(u) - V(u) \times W'(u)}{W^2(u)}, \quad (A.6)$$ 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 $u \to 0$, 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 $u \to \infty$, one has: $W^2 \approx A^2 u^{2B}$ and $u[V' \times W - V \times W'] \approx \frac{2}{3} a u^{2/3} A^2 u^{2B}$, and therefore, in this highly degenerate case and at T=0K,

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

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

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

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

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

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

In particular, in the following, $m^*_{n(p)}/m_o = m_r/m_o$, is taken to culculate the band gap narrowing (BGN), as used in Sections 3 and 5. Therefore, the correlation energy of an effective electron gas, $E_{CE}\left(r_{sn(sp)}\right)$, is found to be given by [1]:

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

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

$$\Delta E_{gn}(N^*, r_d) \simeq a_1 \times \frac{\varepsilon_o}{\varepsilon(r_d)} \times N_r^{1/3} + a_2 \times \frac{\varepsilon_o}{\varepsilon(r_d)} \times N_r^{\frac{1}{3}} \times (2.503 \times [-E_{CE}(r_{sn}) \times r_{sn}]) + a_3 \times \left[\frac{\varepsilon_o}{\varepsilon(r_d)}\right]^{5/4} \times \sqrt{\frac{m_p}{m_r}} \times$$
$$N_r^{1/4} + a_4 \times \sqrt{\frac{\varepsilon_o}{\varepsilon(r_d)}} \times N_r^{1/2} \times 2 + a_5 \times \left[\frac{\varepsilon_o}{\varepsilon(r_d)}\right]^{\frac{3}{2}} \times N_r^{\frac{1}{6}},\ N_r \equiv \frac{N^*=N-N_{CDn}(r_d)}{9.999\times 10^{17}\,cm^{-3}}, \quad \text{(B3)}$$

and

$$\Delta \mathbb{E}_{gp}(N^*, r_a) \simeq a_1 \times \frac{\varepsilon_o}{\varepsilon(r_a)} \times N_r^{1/3} + a_2 \times \frac{\varepsilon_o}{\varepsilon(r_a)} \times N_r^{\frac{1}{3}} \times \left(2.503 \times [-E_{CE}\left(r_{sp}\right) \times r_{sp}]\right) + a_3 \times \left[\frac{\varepsilon_o}{\varepsilon(r_a)}\right]^{5/4} \times \sqrt{\frac{m_n}{m_r}} \times$$
$$N_r^{1/4} + 2a_4 \times \sqrt{\frac{\varepsilon_o}{\varepsilon(r_a)}} \times N_r^{1/2} + a_5 \times \left[\frac{\varepsilon_o}{\varepsilon(r_a)}\right]^{\frac{3}{2}} \times N_r^{\frac{1}{6}},\ N_r \equiv \left(\frac{N^*=N-N_{CDp}(r_a)}{9.999\times 10^{17}\ cm^{-3}}\right), \quad \text{(B4)}$$

Here, $\varepsilon_o = 15.69$, $a_1 = 3.80 \times 10^{-3}(eV)$, $a_2 = 6.5 \times 10^{-4}(eV)$, $a_3 = 2.85 \times 10^{-3}(eV)$, $a_4 = 5.597 \times 10^{-3}(eV)$ and $a_5 = 8.1 \times 10^{-4}(eV)$.

Therefore, in Equations (B3, B4), at T=0 K and $N^* = 0$, and for any $r_{d(a)}$, $\Delta \mathbb{E}_{gn(gp)}(N^* = 0, r_{d(a)}) = 0$, according to the metal-insulator transition (MIT).

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