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Same maximum figure of merit ZT(=1), due to effects of impurity size and heavy doping, obtained in the n(p)-type degenerate Si-crystal ($\xi_{n(p)}(\geqq 1)$), at same reduced Fermi energy $\xi_{n(p)}(=1.813)$ and same minimum (maximum) Seebeck coefficient $Sb\left(=(\mp)1.563\times10^{-4}\frac{V}{K}\right)$, at which same $(ZT)_{Mott}(=\frac{\pi^2}{3\times\xi^2_{n(p)}}\simeq 1)$

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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 Si 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, $N^{EBT}_{CDn(CDp)}(r_{d(a)})$, given in Eq. (21).

(2) In Table 5, the numerical results of the electrical conductivity, $\sigma(N^*, r_{d(a)}, T)$, given in Eq. (27), are obtained for the degenerate P-Si system, suggesting an accuracy of the order of 7.5%, which gives us confidence in the determination of other electrical-and-thermoelectric properties.

(3) Finally, in Tables 10 and 11, 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 Sb present a same minimum (maximum) $\left(=(\mp)1.563\times10^{-4}\frac{V}{K}\right)$, those of the figure of merit ZT show a same maximum $ZT(=\mathbf{1})$, **(ii)** for $\xi_n=1$, those of Sb and those of ZT present same results: $Sb\left(=(\mp)1.322\times10^{-4}\frac{V}{K}\right)$ 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 $(ZT)_{Mott}=\frac{\pi^2}{3\times\xi_{n(p)}^2}(\simeq 1$ and 3.290), respectively, and finally, **(iv)** we show here that in the degenerate Si-case, the Wiedemann-Frank, 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 Si 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, 5, 6] are presented in Tables 1 and 2. In Section 3, the values of optical band gap are given in Table 3, and also compared with experimental results [8]. 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, $\sigma_{n(p)}$, 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 Si-crystal, such as: (i) if denoting the free electron mass by m_o, the relative effective electron (hole) mass,

$m^*_{n(p)}/m_o$, which is equal to the relative effective mass, $m_{n(p)}/m_o$ [5], as used in this Sections 2 and 4 to determine the critical impurity density in the MIT, (ii) to the reduced effective mas, $m_r = \frac{m_n \times m_p}{m_n + m_p} \times m_o$, as used in Section 3 to determine the optical band gap (**OBG**), and (iii), to the conductivity effective mass, $m_{Cn(Cp)}/m_o$ [4], as used in Section 5 to determine the electrical-and-thermoelectric coefficients. Further, $\mathbb{E}_{go}(r_{d(a)} = r_{Si})$ [4] is the unperturbed intrinsic band gap, as used in Section 3 to determine the optical band gap, ε_o [4], is the relative intrinsic dielectric constant, the critical impurity density in the MIT, $N_{CDn(CDp)}(r_{P(B)})$ [2, 6], and finally, the effective averaged numbers of equivalent conduction (valence)-band edge, $g_{c(v)} = 3(2)$ [2, 6], used for present majority-carrier transport phenomena, instead of those, equal to: 6(2), used for other minority-carrier transport phenomena [7].

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.

$m_{n(p)}/m_o$ [5]	m_r/m_o [5]	$m_{Cn(Cp)}/m_o$ [4]	$g_{c(v)}$ [2, 6]	$\mathbb{E}_{go}$ [4]	ε_o [4]	$N_{CDn(CDp)}(r_{P(B)})$ [2, 6]
0.3216(0.3664)	0.1713	0.26(0.373)	3(2)	1.17 eV	11.4	$3.52\ (4.06) \times 10^{18}$ cm^{-3}

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 MIT, as follows.

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

In the [d(a)-semiconductors]-systems, since $r_{d(a)}$, given in tetrahedral covalent bonds, is usually either larger or smaller than $r_{do(ao)} \equiv r_{Si}$, a local mechanical strain (or deformation potential energy) is induced, according to a compression (dilation) for: $r_{d(a)} > r_{do(ao)}$ ($r_{d(a)} < r_{do(ao)}$), due to the d(a)-size effect, respectively [1]. 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 shown [1] that, as $r_{d(a)} > r_{do(ao)}$ ($r_{d(a)} < r_{do(ao)}$), such the compression (dilatation) corresponding the repulsive (attractive) force increases (decreases) the intrinsic energy gap $\mathbb{E}_{gni(gpi)}(r_{d(a)})$ and the effective donor(acceptor)-ionization energy $\mathbb{E}_{d(a)}(r_{d(a)})$ in absolute values, obtained in an effective Bohr model, as [1]:

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

where

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

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

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

2.2. Our expressions for the critical density in the MIT

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

$$N_{CDn(NDp)}(r_{d(a)})^{1/3}\times a_{Bn(Bp)}(r_{d(a)})=z,\ z=0.290364495(0.3687017088), \quad (3)$$

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

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

where $-q$ is the electron charge, $\varepsilon(r_{d(a)})$ is determined in Eq. (2), and $m^*_{n(p)}/m_o=m_{n(p)}/m_o=0.3216(0.3664)$, as given in Table 1. It should be noted in Eq. (3) that, for the Mott criterion in the MIT, z_{Mott}=0.25, while in the present work, z=0.290364495(0.3687017088), is chosen so that we can obtain the exact values of $N_{CDn(CDp)}(r_{P(B)})=3.52\ (4.06)\times10^{18}\ \text{cm}^{-3}$ [2, 6], as those given in Table 1. Further, these obtained results can also be justified by those of the densities of electrons (holes) localized in exponential conduction (valance)-band (EBT) tails, $N^{EBT}_{CDn(CDp)}(r_{P(B)})\equiv N_{CDn(CDp)}(r_{P(B)})=3.52\ (4.06)\times10^{18}\ \text{cm}^{-3}$, obtained using Eq. (21), as investigated in Section 4, and reported also in Table 2. In this Table, we also present various values of $\varepsilon(r_{d(a)})$, $a_{Bn(Bp)}(r_{d(a)})$, $\mathbb{E}_{d(a)}(r_{d(a)})$ and $\mathbb{E}_{gni(gpi)}(r_{d(a)})$, $N_{CDn(NDp)}(r_{d(a)})$, and $N^{EBT}_{CDn(CDp)}(r_{d(a)})$, noting that the maximal relative deviations, in absolute values, $|RD|$, between $N_{CDn(NDp)}(r_{d(a)})$ and $N^{EBT}_{CDn(CDp)}(r_{d(Ba)})$ are found to be equal to: $9.8(4.91)\times10^{-6}$, respectively. In other word, $N_{CDn(NDp)}(r_{d(a)})$, determined in Eq. (3), can be explained by the densities of electrons (holes) localized in exponential conduction (valance)-band (EBT) tails, $N^{EBT}_{CDn(CDp)}(r_{d(a)})$, determined in Eq. (21). Furthermore, in our recent work [6], we showed that, in the n(p)-type degenerate Si, the critical densities of electrons (holes) can also be determined from the spin-susceptibility singularities (SSS), obtained at $N=N^{SSS}_{CDn(CDp)}(r_{d(a)})$, at which the MITs occur.

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

Donor		P	Si	As	Te	Sb	Sn
r_d (nm) [4]	↗	0.110	0.117	0.118	0.132	0.136	0.140
$\varepsilon(r_d)$	↘	11.58	11.4	11.396	10.59	10.16	9.69
$a_{Bn}(r_d)$ in nm	↘	1.91	1.88	1.878	1.75	1.67	1.60
$\mathbb{E}_d(r_d)$ in meV	↗	32.6	33.7	33.7	39.0	42.3	46.6
$\mathbb{E}_{gni}(r_d)$ in meV	↗	1168.9	1170	1170.02	1175.04	1178.67	1182.9
$N_{CDn}(r_d)$ in 10^{18} cm^{-3}	↗	3.52 [6]	3.69181	3.69547	4.59924	5.20648	6.01115

$N_{CDn}^{EBT}(r_d)$ in 10^{18} cm^{-3}	↗	3.52 [6]	3.69179	3.695468	4.599223	5.20643	6.01109
|RD| in 10^{-6}		0	6.5	0.4	3.7	**9.8**	9.4

Acceptor		**B**	**Si**	**Ga(Al)**	**Mg**	**In**
r_a (nm) [4]	↗	0.088	0.117	0.126	0.140	0.144
$\varepsilon(r_a)$	↘	15.98	11.4	11.1	9.69	9.19
$a_{Bp}(r_a)$ in nm	↘	2.31	1.65	1.60	1.40	1.33
$\mathbb{E}_a(r_a)$ in meV	↗	19.5	38.3	40.5	53.1	59.0
$\mathbb{E}_{gpi}(r_a)$ in meV	↗	1151.2	1170	1172.1	1184.7	1190.6
$N_{CDp}(r_a)$ in 10^{18} cm^{-3}	↗	4.06 [6]	11.177705	12.118516	18.199979	21.328851
$N_{CDp}^{EBT}(r_a)$ in 10^{18} cm^{-3}	↗	4.06 [6]	11.177737	12.118572	18.199970	21.328810
|RD| in 10^{-6}		0	2.8	4.58	**4.91**	1.95

Table 2 also indicates that, for increasing $r_{d(a)}$, both $\varepsilon(r_{d(a)})$ and $a_{Bn(Bp)}(r_{d(a)})$ decrease, while $\mathbb{E}_{d(a)}(r_{d(a)})$, $\mathbb{E}_{gni(gpi)}(r_{d(a)})$, $N_{CDn(NDp)}(r_{d(a)})$ and $N_{CDn(CDp)}^{EBT}(r_{d(a)})$ increase, affecting strongly all the physical properties, as those given in following Sections 3-5 .

3. Optical band gap

Here, $m_{n(p)}^*/m_o$ is chosen as: $m_{n(p)}^*/m_o = m_r/m_o = 0.1713$, and then, if denoting $N^* \equiv N - N_{CDn(NDp)}(r_{d(a)})$, the optical band gap (**OBG**) is found to be given by:

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

where the reduced band gap is defined as:

$$\mathbb{E}_{gn2(gp2)}(N^*, r_{d(a)}, T) \equiv \mathbb{E}_{gni(gpi)}(r_{d(a)}) - 0.071\text{eV} \times \left\{\left(1 + \left[\frac{2T}{440.6913}\right]^{2.201}\right)^{\frac{1}{2.201}} - 1\right\} - \Delta\mathbb{E}_{gn(gp)}(N^*, r_{d(a)}).$$

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

Finally, the numerical results of $\mathbb{E}_{gn1(gp1)}(N^* > 0, r_{d(a)}, T)$ at T=20K, calculated using Eq. (5), expressed as functions of N and $r_{d(a)}$, and reported in Table 3, being also compared with the corresponding data [8], obtained in the P(B)-type degenerate Si, giving rise to the accuracies of the order of 1.16% (2.68%), respectively.

Table 3. In degenerate d(a)-Si systems at T=20K, the numerical results of the OBG, evaluated using Eq. (5), and in P(B)-systems, those also compared with corresponding $\mathbb{E}_{gn1}^{Data}$ [8], giving rise to the relative deviations in absolute values |RD|, 1.16% and 2.68%, respectively.

N (10^{18} cm^{-3})	4	8.5	15	50	80	150
$\mathbb{E}_{gn1}^{Data}(N^*, r_P)$ in eV [8]	1.138	1.133	1.129	1.131	1.132	1.133
$\mathbb{E}_{gn1}(N^*, r_P)$ in eV	1.149	1.129	1.121	1.118	1.124	1.146
|RD| in (%)	0.9	0.3	0.6	**1.16**	0.7	1.15
$\mathbb{E}_{gn1}(N^*, r_{As})$ in eV	1.152	1.130	1.121	1.117	1.123	1.144
$\mathbb{E}_{gn1}(N^*, r_{Te})$ in eV		1.133	1.122	1.113	1.117	1.134
$\mathbb{E}_{gn1}(N^*, r_{Sb})$ in eV		1.136	1.123	1.111	1.113	1.129
$\mathbb{E}_{gn1}(N^*, r_{Sn})$ in eV		1.142	1.125	1.108	1.109	1.122
N (10^{18} cm^{-3})	6.5	11	15	26	60	170
$\mathbb{E}_{gp1}^{Data}(N^*, r_B)$ in (eV) [8]	1.142	1.140	1.139	1.142	1.142	1.162
$\mathbb{E}_{gp1}(N^*, r_B)$ in eV	1.120	1.113	1.111	1.112	1.127	1.193
|RD| in (%)	1.9	2.3	2.4	2.64	1.3	**2.68**
$\mathbb{E}_{gp1}(N^*, r_{Ga(Al)})$ in eV			1.121	1.098	1.088	1.119
$\mathbb{E}_{gp1}(N^*, r_{Mg})$ in eV				1.107	1.077	1.089
$\mathbb{E}_{gp1}(N^*, r_{In})$ in eV				1.118	1.074	1.078

Furthermore, in Table 3, we also showed that, in the n(p)-type degenerate Si 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 $(E - \mathbb{E}_{gn1(gp1)})^2$. Therefore, if the values of $\mathbb{E}_{gn1(gp1)}$ obtained in Table 3 increase (decrease), $(E - \mathbb{E}_{gn})^2$ and other optical coefficients then decrease (increase), respectively.

4. Physical model and mathematical methods

4.1. Physical model

In the n(p)-type degenerate Si, 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

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

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

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

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 $R_{snTF(snTF)}$ is reduced to

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

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

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

$$R_{sn(sp)WS}\left(N^{*}, r_{d(a)}\right) \equiv \frac{k_{sn(sp)WS}}{k_{Fn}} = 1(0.389856828) \times \left(\frac{3}{2\pi} - \gamma \frac{d\left[r_{sn(sp)}^{2} \times \mathbb{E}_{CE}\left(N^{*}, r_{d(a)}\right)\right]}{dr_{sn(sp)}}\right), \quad (9)$$

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

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

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)-Si 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 Si crystal, is defined by

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

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)-Si system, defined as

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

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 $\vec{k}$-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 Si-crystal volume.

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

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

Here, $\varepsilon(r_{d(a)})$ is determined in Eq. (2), $R_{sn(sp)}(N^*, r_{d(a)})$in Eq. (7), the empirical Heisenberg parameter $\mathcal{H} = 3.320313702$ 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 $\mathbb{E}_{Fno(Fpo)}$ 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 $W_{n(p)}(\nu_{n(p)}, N^*, r_{d(a)})$.

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

A. Kane integration method (KIM)

In heavily doped d(a)-Si 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

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

noting that as a=1, $(it)^{-\frac{3}{2}} \times \exp\left\{-\frac{(t\sqrt{W_p})^2}{2\hbar^2}\right\}$ is found to be proportional to the averaged Feynman propagator given the dense donors(acceptors).

Then, by variable changes: $t = \frac{\hbar}{\sqrt{W_{n(p)}}}$ and $x = -\mathbb{E}/\sqrt{W_{n(p)}}$, 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) $\underline{\mathbb{E}\geq 0}$-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 $\underline{\mathbb{E}\geq 0}$, 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:

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

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

C. Critical impurity density in the MIT

In degenerate d(a)-Si systems at T=0 K, in which $m^*_{n(p)}/m_o = m_{n(p)}/m_o = 0.3216(0.3664)$, as given in Table 1, using Eq. (13), for a=1, the density of states $\mathcal{D}(\mathbb{E})$ is defined by:

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

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

Here, $\mathbb{E}_{Fno}$ is determined in Eq. (A4) of the Appendix A, with $m^*_{n(p)}/m_o = m_{n(p)}/m_o$ and $\mathcal{H} = 3.320313702$, being chosen such that the following determination of $N^{EBT}_{CDn(CDp)}(N, r_{d(a)})$ 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:

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

(19)

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

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

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

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

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

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

Finally, Eq. (20) now yields:

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

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

The numerical results of $N_{CDn(CDp)}^{EBT}(N, r_{d(a)})$, evaluated using Eq. (21), are given in Table 2, confirming thus those of $N_{CDn(NDp)}(r_{d(a)})$, calculated using Eq. (3).

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:

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

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

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

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

$I_{2n} = 2 \int_0^{\infty} \frac{\gamma^{2n} \times e^{\gamma}}{(1+e^{\gamma})^2} d\gamma$. (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: $I_{2n} = \left(2^{2n} - 2\right) \times \pi^{2n} \times |B_{2n}|$. So, from Eq. (22), we get in the degenerate case the following ratio:

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

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 $G_{p=1}(y \equiv \frac{\pi k_B T}{\mathbb{E}_{Fn(Fp)}} = \frac{\pi}{\xi_{n(p)}}) = 1$, 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 Si, in the following.

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

Here, $m^*_{n(p)}/m_o$ is chosen as: $m^*_{n(p)}/m_o = m_{Cn(Cp)}/m_o = 0.26(0.373)$, 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:

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

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:

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

which is thus proportional to $\mathbb{E}_k{}^2$, $C = (0.89645)^2$ being chosen such that the numerical results of σ will be in good accordance with the corresponding experimental ones [9, 10]. 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:

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

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 $\mathbb{E}_{Fn(Fp)}$ and $\mathbb{E}_{Fno(Fpo)}$ 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. Then, in the degenerate P-Si system at T=4.2 K and T=77 K, the numerical results of ρ and σ are calculated, using Eq. (27), and reported also in Table 5, suggesting maximal relative errors of the order of 13.178% (7.5%), respectively. Such an accuracy of $\sigma(N^*, r_{d(a)}, T)$ gives us a good confidence, using Eq. (27) to determine other electrical-and-thermoelectric properties, in the following.

Table 5. In the degenerate P-Si system, our numerical results of resistivity $\rho(N^*)$ and conductivity $\sigma(N^*)$, calculated using Eq. (27), are obtained respectively at 4.2K and 77K, respectively, accompanied by their relative deviations in absolute values, $|RD|$, calculated, using the corresponding data [9, 10].

$N\ (10^{19}\ cm^{-3})$	1.1	1.6	2.7	3.9	7	13
The following resistivity results obtained at T=**4.2K** are expressed in 10^{-4} ohm × cm.						
ρ_{data} [9]	33	23	13	9.4	6	3.8
ρ (|RD|)	37.3(**13.178%**)	24.4 (5.9%)	14.29 (9.9%)	10.02 (6.7%)	5.82 (3%)	3.3 (13.173%)

$N\ (10^{19}\ cm^{-3})$	1.85	5.55	8.65
The following conductivity results obtained at T=**77K** are expressed in $\text{ohm}^{-1} \times \text{cm}^{-1}$.			
σ_{data} [10]	559	1500	2000
σ (|RD|)	517 (**7.5%**)	1409 (6.1**%**)	2105 (5.2%)

A.Electrical properties

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

$\tau(N^*, r_{d(a)}, T) \equiv \sigma(N^*, r_{d(a)}, T) \times \frac{m_{Cn(Cp)}}{q^2 \times N^*}$. 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.

Now, in the degenerate d(a)-Si systems, at T=4.2 K and T=77 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 6 and 7.

Table 6. 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 $\left(\frac{1}{ohm \times cm}, \frac{cm^2}{V \times s}, \frac{cm^2}{V \times s}, \frac{cm^2}{s}\right)$					
N(10^{19} cm^{-3})					
3	775, 183, 183, 7.3	752, 178, 178, 7.1	651, 160, 160, 6.2	599, 151, 151, 5.8	541, 141, 141, 5.3
10	2384, 154, 154, 14.6	2317, 150, 150, 14.2	2039, 133, 133, 12.5	1896, 125, 125, 11.7	1741, 116, 116, 10.5
40	8487, 134, 134, 32.4	8248, 130, 130, 31.5	7256, 114, 114, 27.7	6749, 107,107, 25.8	6207, 98, 98, 23.7
70	14227, 127, 127, 45.0	13823, 124, 124, 43.74	12146, 109, 109, 38.4	11290, 101, 101, 35.7	10375, 93, 93, 32.9
100	19809, 124, 124, 55.6	19243, 120, 120, 54.0	16894, 106, 106, 47.4	15696, 98, 98, 44.1	14417, 90, 90, 40.5
In the following, our numerical results of (σ, μ, μ_H, D) at **77**K, expressed respectively in $\left(\frac{1}{ohm \times cm}, \frac{cm^2}{V \times s}, \frac{cm^2}{V \times s}, \frac{cm^2}{s}\right)$					
N(10^{19} cm^{-3})					
3	806, 190, 218, 7.8	781, 185, 213, 7.6	678, 167, 193, 6.6	624, 157, 183, 6.2	565, 147, 172, 5.7
10	2401, 155, 160, 14.7	2334, 151, 155, 14.3	2054, 134, 138, 12.7	1910, 126, 129, 11.8	1754, 116, 120, 10.9
40	8496, 134, 134, 32.5	8257, 130, 131, 31.5	7264, 115, 115, 27.8	6757, 107, 107, 25.8	6214, 98, 99, 23.8
70	14234, 127, 128, 45.0	13830, 124, 124, 43.8	12152, 109, 109, 38.5	11296, 101, 102, 35.8	10381, 93, 93, 32.9
100	19817, 124, 124, 52.6	19249, 120, 121, 54.1	16900, 106, 106, 47.5	15701, 98, 99, 44.1	14421, 90, 91, 40.5

Table 7. 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	B	Ga(Al)	Mg	In
In the following, our numerical results of (σ, μ, μ_H, D) at 4.2K, expressed respectively in $\left(\frac{1}{\text{ohm}\times\text{cm}}, \frac{\text{cm}^2}{\text{V}\times\text{s}}, \frac{\text{cm}^2}{\text{V}\times\text{s}}, \frac{\text{cm}^2}{\text{s}}\right)$				
$N(10^{19}\ \text{cm}^{-3})$				
3	1577, 379, 380, 13.6	745, 260, 260, 7.3	466, 247, 247, 5.2	348, 251, 251, 4.3
10	4549, 296, 296, 25.4	2504, 178, 178, 14.4	1973,150, 151, 11.6	1787, 142, 142, 10.7
40	13358, 242, 242, 53.6	8450, 136, 136, 29.7	6789, 111, 111, 24.0	6234, 103, 103, 22.1
70	25315, 227, 227, 73.2	13794, 125, 125, 40.0	11060, 101, 101, 32.2	10152, 93, 93, 29.6
100	34908, 219, 219, 89.5	18896, 119, 119, 48.6	15117, 96, 96, 39.0	13867, 88, 88, 35.8
In the following, our numerical results of (σ, μ, μ_H, D) at **77**K, expressed respectively in $\left(\frac{1}{\text{ohm}\times\text{cm}}, \frac{\text{cm}^2}{\text{V}\times\text{s}}, \frac{\text{cm}^2}{\text{V}\times\text{s}}, \frac{\text{cm}^2}{\text{s}}\right)$				
$N(10^{19}\ \text{cm}^{-3})$				
3	1652, 397, 469, 14.8	802, 280, 359, 8.3	526, 278, 402, 6.5	416, 299, 488, 5.8
10	4588, 298, 309, 25.8	2529, 179, 186, 14.7	1994, 152, 159, 11.8	1807, 143, 150, 10.9
40	15378, 242, 244, 53.7	8462, 136, 137, 29.7	6799, 111, 112, 20.0	6242, 103, 103, 22.1
70	25331, 227, 228, 73.2	13803, 125, 125, 40.1	11067, 101, 101, 32.2	10158, 93, 94, 29.6
100	34922, 219, 219, 89.6	18903, 119, 120, 48.6	15123, 96, 96, 39.0	13872, 88, 89, 35.8

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, Sb, is given in the n(p)-type degenerate Si, as:

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

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

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

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:

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

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

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

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

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

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

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

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

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)-Si, defined by physical conditions : $N = 10^{21} cm^{-3}$ and T (=3K and 300K), the numerical results of $\xi_{n(p)} \equiv \frac{\mathbb{E}_{Fn(Fp)}(N^*,T)}{k_B T}$, 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), $Sb(N^*,T)$, $Ts(N^*,T)$, $Pt(N^*,T)$ 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 8 and 9.

Table 8. 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} cm^{-3}) is very high, N^* therefore decreases slowly, explaining the slow decrease (↘) in $\frac{\mathbb{E}_{Fn}(N^*,T=300K)}{k_B T}$, σ, κ, C_κ, and $\kappa_{App.}$, (ii) the numerical result: $\left|RD_{\kappa,\kappa_{App.}}\right|_{300K} \simeq 4.84 \times 10^{-3}$ 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 Si-case the well-known Wiedemann-Frank, given in Eq. (25a), is found to be exact.

Donor	P	As	Te	Sb	Sn
Highly degenerate d-Si systems for N=10^{21} cm^{-3} and at T=3K and T=300K, noting that $N^* \equiv N - N_{CDn}(r_d)$					
$\frac{\mathbb{E}_{Fn}(N^*,T=300K)}{k_B T} \gg 1$ ↘	26.06	26.06	26.04	26.03	26.01
$\sigma_{(T=3K)}\ \left(\frac{10^4}{ohm \times cm}\right)$ ↘	1.9809	1.9243	1.6894	1.5696	1.4417
$\sigma_{(T=300K)}\ \left(\frac{10^4}{ohm \times cm}\right)$ ↘	1.9905	1.9336	1.6976	1.5772	1.4487
$\kappa_{(T=3K)}\ \left(\frac{10^{-3} \times W}{cm \times K}\right)$ ↘	1.4518	1.4103	1.2382	1.1504	1.0566
$\kappa_{(T=300K)}\ \left(\frac{W}{cm \times K}\right)$ ↘	0.1459	0.1417	0.1244	0.1156	0.1062
$C_\kappa\ \left(\frac{10^{-5} \times W}{cm \times K^2}\right)$ ↘	48.3936	47.0097	41.2721	38.3456	35.2199
$\kappa_{App.}(300K)\ \left(\frac{W}{cm \times K}\right)$ ↘	0.1452	0.1410	0.1238	0.1150	0.1056
$\left\|RD_{\kappa,\kappa_{App.}}\right\|_{300K}$ in 10^{-3}	4.821	4.822	4.828	4.831	4.837
$Sb_{(T=3K)}\ \left(\frac{10^{-7} \times V}{K}\right)$	−2.180	−2.180	−2.181	−2.182	−2.183

$Sb_{(T=300K)}\ (\frac{10^{-5}\times V}{K})$	-2.165	-2.165	-2.167	-2.168	-2.169
$Ts_{(T=3K)}\ (\frac{10^{-7}\times V}{K})$	-2.180	-2.180	-2.181	-2.182	-2.183
$Ts_{(T=300K)}\ (\frac{10^{-5}\times V}{K})$	-2.136	-2.137	-2.138	-2.139	-2.140
$Pt_{(T=3K)}\ (10^{-7}\times V\ )$	-6.539	-6.540	-6.544	-6.547	-6.550
$Pt_{(T=300K)}\ (10^{-3}\times V\ )$	-6.496	-6.497	-6.500	-6.503	-6.507
$ZT_{(T=3K)}\ (\times 10^{-6})$	1.945	1.945	1.948	1.949	1.951
$ZT_{(T=300K)}(\times 10^{-2}\ )$	1.919	1.920	1.922	1.923	1.925
$\lvert RD_{L,L_{VC}}\rvert$ in 10^{-6} at 3 K	1.534	1.534	1.534	1.534	**1.534**
$\lvert RD\rvert$ in 10^{-6} at 300K	1.535	1.535	1.535	1.535	**1.535**

Table 9. 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} 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: $\left|RD_{\kappa,\kappa_{App.}}\right|_{300K} \simeq 4.84\times 10^{-3}$ 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 Si-case the well-known Wiedemann-Frank, given in Eq. (25a), is found to be exact.

Acceptor		B	Ga (Al)	Mg	In
Highly degenerate a-Si systems for N=10^{21} cm^{-3} and T=3K and T=300K					
$\frac{\mathbb{E}_{Fp}(N^*,T=300K)}{k_BT} \gg 1$	↘	23.80	23.67	23.58	23.53
$\sigma_{(T=3K)}\ (\frac{10^4}{ohm\times cm})$	↘	3.4908	1.8896	1.5117	1.3867
$\sigma_{(T=300K)}\ (\frac{10^4}{ohm\times cm})$	↘	3.5111	1.9007	1.5207	1.3949
$\kappa_{(T=3K)}\ (\frac{10^{-3}\times W}{cm\times K})$	↘	2.5584	1.3848	1.1079	1.0163
$\kappa_{(T=300K)}\ (\frac{W}{cm\times K})$	↘	0.2573	0.1393	0.1114	0.1022
$C_\kappa\ (\frac{10^{-5}\times W}{cm\times K^2})$ at T=3K	↘	85.2802	46.1616	36.9315	33.8767
$\kappa_{App.}(300K)\ (\frac{W}{cm\times K})$	↘	0.2558	0.1385	0.1108	0.1016
$\left\lvert RD_{\kappa,\kappa_{App.}}\right\rvert_{300K}$ in 10^{-3}		5.773	5.835	5883	5.907
$Sb_{(T=3K)}(\frac{10^{-7}\times V}{K})$		2.387	2.400	2.410	2.415
$Sb_{(T=300K)}\ (\frac{10^{-5}\times V}{K})$	2.368	2.381	2.391	2.396	
$Ts_{(T=3K)}\ (\frac{10^{-7}\times V}{K})$		2.387	2.400	2.410	2.415
$Ts_{(T=300K)}\ (\frac{10^{-5}\times V}{K})$		2.331	2.343	2.352	2.357
$Pt_{(T=3K)}\ (10^{-7}\times V\ )$		7.162	7.201	7.230	7.246
$Pt_{(T=300K)}\ (10^{-3}\times V\ )$		7.105	7.143	7.172	7.187
$ZT_{(T=3K)}\ (\times 10^{-6})$		2.333	2.358	2.378	2.388
$ZT_{(T=300K)}(\times 10^{-2}\ )$		2.296	2.320	2.339	2.349
$\lvert RD_{L,L_{VC}}\rvert$ in 10^{-6} at 3 K		1.534	1.534	1.534	**1.534**
$\lvert RD_{L,L_{VC}}\rvert$ in 10^{-6} at 300 K		1.535	1.535	1.535	**1.535**

Secondly, in the highly degenerate d(a)-Si, for a given N^*, the values of $\xi_{n(p)} \equiv \frac{\mathbb{E}_{Fn(Fp)}(N^*,T)}{k_B T}$, calculated by using Eq. (A3) of the Appendix A, and other ones of: $Sb(N^*,T)$ by Eq. (30), $\left|RD_{L,L_{VC}}\right|$ 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 10 and 11.

Table 10. Here, for a given N^* and for a given degenerate d-Si 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 $\xi_n = 1.813$, while the numerical results of Sb present a same minimum $(Sb)_{min.}\left(=-1.563\times10^{-4}\frac{V}{K}\right)$, those of ZT show a same maximum $ZT_{max.}(=\mathbf{1})$, (ii) for $\xi_n = 1$, Sb and ZT present same results: $-1.322\times10^{-4}\frac{V}{K}$ 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: $\simeq 1$ 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 Si-case the Wiedemann-Frank, given in Eq. (25a), is exact.

In the degenerate P-Si system, $N^* \equiv N - N_{CDn}(r_P) \equiv (5.962-3.52)\times10^{18}\ cm^{-3} \equiv 2.442\times10^{18}\ cm^{-3}$												
T(K)	↗	40		50		**63.945**		70		**87.00367**		88
ξ_n	↘	3.663		2.677		**1.813**		1.552		**1**		0.973
$Sb\left(10^{-4}\frac{V}{K}\right)$		−1.243	↘	−1.451	↘	**−1.563**	↗	−1.544	↗	**− 1.322**	↗	− 1.302
$\left\|RD_{L,L_{VC}}\right\|$ in 10^{-6}		1.539		1.540		1.541		1.541		1.539		1.540
ZT		0.632	↗	0.862	↗	**1**	↘	0.976	↘	**0.715**	↘	0.694
$(ZT)_{Mott} = \frac{\pi^2}{3\times\xi_n^2}$	↗	0.245		0.459		**1.0004**		1.366		3.290		3.472
$T_s\left(10^{-8}\frac{V}{K}\right)$	↗	−9423		−8160		5.129		4256		16574		17258
Pt $(10^{-3}V)$		− 4.972	↘	−7.258	↘	−9.994	↘	−10.81	↘	−11.50	↗	−11.461
In the degenerate As-Si system, $N^* \equiv N - N_{CDn}(r_{As}) \equiv (6.238-3.695)\times10^{18}\ cm^{-3} \equiv 2.542\times10^{18}\ cm^{-3}$												
T(K)	↗	41		51		**65.672**		70		**89.3753**		90
ξ_n	↘	3.673		2.706		**1.813**		1.627		**1**		0.984
$Sb\left(10^{-4}\frac{V}{K}\right)$		−1.241	↘	−1.446	↘	**−1.563**	↗	−1.554	↗	**−1.322**	↗	−1.310
$\left\|RD_{L,L_{VC}}\right\|$ in 10^{-6}		1.539		1.540		1.541		1.541		1.540		1.540
ZT		0.630	↗	0.855	↗	**1**	↘	0.988	↘	**0.715**	↘	0.702
$(ZT)_{Mott} = \frac{\pi^2}{3\times\xi_n^2}$	↗	0.244		0.449		**0.9996**		1.242		3.290		3.400
$Ts\left(10^{-8}\frac{V}{K}\right)$	↗	−9407		−8305		−5.554		2928		16574		16993
Pt $(10^{-3}V)$		− 5.088	↘	−7.373	↘	−10.264	↘	−10.87	↗	−8.313	↗	−11.79
In the degenerate Te-Si system, $N^* \equiv N - N_{CDn}(r_{Te}) \equiv (7.24-4.599)\times10^{18}\ cm^{-3} \equiv 2.641\times10^{18}\ cm^{-3}$												
T(K)	↗	42		52		**67.37**		71		**91.66275**		92
ξ_n	↘	3.678		2.730		**1.813**		1.659		**1**		0.991
$Sb\left(10^{-4}\frac{V}{K}\right)$		−1.240	↘	−1.441	↘	**−1.563**	↗	−1.557	↗	**−1.322**	↗	−1.315
$\left\|RD_{L,L_{VC}}\right\|$ in 10^{-6}		1.539		1.540		1.541		1.541		1.540		1.540
ZT		0.629	↗	0.850	↗	**1**	↘	0.992	↘	**0.715**	↘	0.708
$(ZT)_{Mott} = \frac{\pi^2}{3\times\xi_n^2}$	↗	0.243		0.441		**1.0004**		1.195		3.290		3.347
$Ts\left(10^{-8}\frac{V}{K}\right)$	↗	−9398		−8420		5.574		2396		16574		16795
Pt $(10^{-3}V)$		− 5.208	↘	−7.49	↘	−10.53	↘	−11.05	↘	−12.11	↗	−12.10
In the degenerate Sb-Si system, $N^* \equiv N - N_{CDn}(r_{Sb}) \equiv (8.208-5.206)\times10^{18}\ cm^{-3} \equiv 3.001\times10^{18}\ cm^{-3}$												
T(K)	↗	52		62		**73.37**		81		**99.8315**		100
ξ_n	↘	3.096		2.376		**1.813**		1.529		**1**		0.996
$Sb\left(10^{-4}\frac{V}{K}\right)$		−1.363	↘	−1.508	↘	**−1.563**	↗	−1.540	↗	**−1.322**	↗	−1.319
$\left\|RD_{L,L_{VC}}\right\|$ in 10^{-6}		1.540		1.540		1.541		1.541		1.540		1.540
ZT		0.761	↗	0.930	↗	**1**	↘	0.971	↘	**0.715**	↘	0.712
$(ZT)_{Mott} = \frac{\pi^2}{3\times\xi_n^2}$	↗	0.343		0.582		**1.0002**		1.408		3.290		3.316
$Ts\left(10^{-8}\frac{V}{K}\right)$	↗	−9545		−6191		3.280		4683		16574		16675
Pt $(10^{-3}V)$		− 7.089	↘	−9.347	↘	−11.47	↘	−12.48	↘	−13.195	↗	−13.189
In the degenerate Sn-Si system, $N^* \equiv N - N_{CDn}(r_{Sn}) \equiv (14.698-6.01115)\times10^{18}\ cm^{-3} \equiv 8.68685\times10^{18}\ cm^{-3}$												
T(K)	↗	60		100		**149**		180		**202.7443**		203

ξ_n	↘	5.737		3.341		**1.813**		1.291		**1**		0.997
Sb $\left(10^{-4}\frac{V}{K}\right)$		−0.898	↘	−1.311	↘	**−1.563**	↗	−1.477	↗	**−1.322**	↗	−1.320
$\left\|RD_{L,L_{VC}}\right\|$ in 10^{-6}		1.538		1.540		1.541		1.540		1.540		1.540
ZT		0.330	↗	0.703	↗	**1**	↘	0.893	↘	**0.715**	↘	0.713
$(ZT)_{Mott}=\frac{\pi^2}{3\times\xi_n^2}$	↗	0.100		0.295		**1.0001**		1.974		3.290		3.309
Ts $\left(10^{-8}\frac{V}{K}\right)$		−6837	↘	−9716	↗	1.980	↗	9551	↗	16574	↗	16650
Pt $(10^{-3}V)$		−5.391	↘	−13.11	↘	−23.29	↘	−26.58	↘	−26.80	↗	−26.79

Table 11. Here, for a given N^* and for a given degenerate a-Si 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: $1.563\times10^{-4}\frac{V}{K}$ and 1, respectively, (ii) for $\xi_p = 1$, Sb and ZT present same results: $1.322\times10^{-4}\frac{V}{K}$ 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: $\simeq 1$ 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 Si-case the Wiedemann-Frank, given in Eq. (25a), is exact.

In the degenerate B-Si system, $N^*\equiv N-N_{CDp}(r_B)\equiv(4.7-4.06)\times10^{18}\ cm^{-3}\equiv6.4\times10^{17}\ cm^{-3}$											
T(K)	↗	15		20		**23.92**		29		**32.545114**		33
ξ_p	↘	3.651		2.416		**1.813**		1.281		**1**		0.967
Sb $\left(10^{-4}\frac{V}{K}\right)$		1.245	↗	1.501	↗	**1.563**	↘	1.473	↘	**1.322**	↘	1.298
$\left\|RD_{L,L_{VC}}\right\|$ in 10^{-6}		1.539		1.540		1.541		1.540		1.540		1.539
ZT		0.635	↗	0.922	↗	**1**	↘	0.888	↘	**0.715**	↘	0.690
$(ZT)_{Mott}=\frac{\pi^2}{3\times\xi_p^2}$	↗	0.247		0.564		**1.0004**		2.003		3.290		3.514
Ts $\left(10^{-8}\frac{V}{K}\right)$	↘	9440		6497		−5.766		−9759		−16574		−17408
Pt $(10^{-3}V)$		1.868	↗	3.002	↗	3.739	↗	4.272	↗	4.301	↘	4.284
In the degenerate Ga(Al)-Si system, $N^*\equiv N-N_{CDp}(r_{Ga(Al)})\equiv(13.2115-12.118516)\times10^{18}\ cm^{-3}\equiv1.093\times10^{18}\ cm^{-3}$											
T(K)	↗	20		30		**34.175**		39		**46.49879**		47
ξ_p	↘	3.967		2.239		**1.813**		1.439		**1**		0.975
Sb $\left(10^{-4}\frac{V}{K}\right)$		1.182	↗	1.529	↗	**1.563**	↘	1.522	↘	**1.322**	↘	1.303
$\left\|RD_{L,L_{VC}}\right\|$ in 10^{-6}		1.539		1.540		1.541		1.540		1.539		1.539
ZT		0.572	↗	0.957	↗	**1**	↘	0.948	↘	**0.715**	↘	0.696
$(ZT)_{Mott}=\frac{\pi^2}{3\times\xi_p^2}$	↗	0.209		0.656		**1.0004**		1.589		3.290		3.461
Ts $\left(10^{-8}\frac{V}{K}\right)$	↘	8851		4997		−4.913		−6415		−16574		−17218
Pt $(10^{-3}V)$		2.364	↗	4.587	↗	5.341	↗	5.936	↗	6.146	↘	6.127
In the degenerate Mg-Si system, $N^*\equiv N-N_{CDp}(r_{Mg})\equiv(19.90075-18.199979)\times10^{18}\ cm^{-3}\equiv1.701\times10^{18}\ cm^{-3}$											
T(K)	↗	20		30		**45.89**		50		**62.44**		63
ξ_p	↘	5.330		3.461		**1.813**		1.565		**1**		0.979
Sb $\left(10^{-4}\frac{V}{K}\right)$		0.953	↗	1.285	↗	**1.563**	↘	1.546	↘	**1.322**	↘	1.307
$\left\|RD_{L,L_{VC}}\right\|$ in 10^{-6}		1.538		1.539		1.540		1.540		1.539		1.539
ZT		0.372	↗	0.676	↗	**1**	↘	0.978	↘	**0.715**	↘	0.699
$(ZT)_{Mott}=\frac{\pi^2}{3\times\xi_p^2}$	↗	0.116		0.275		**1.0003**		1.343		3.290		3.432
Ts $\left(10^{-8}\frac{V}{K}\right)$		7045	↗	9663	↘	−3.724	↘	−4019	↘	−16574	↘	−17111
Pt $(10^{-3}V)$		1.907	↗	3.856	↗	7.172	↗	7.731	↗	8.253	↘	5.098
In the degenerate In-Si system, $N^*\equiv N-N_{CDp}(r_{In})\equiv(25.25693-21.329)\times10^{18}\ cm^{-3}\equiv4.364\times10^{18}\ cm^{-3}$											
T(K)	↗	50		60		**86**		90		**117.03044**		118
ξ_p	↘	3.997		3.167		**1.813**		1.679		**1**		0.981
Sb $\left(10^{-4}\frac{V}{K}\right)$		1.176	↗	1.348	↗	**1.563**	↘	1.558	↘	**1.322**	↘	1.308
$\left\|RD_{L,L_{VC}}\right\|$ in 10^{-6}		1.539		1.539		1.540		1.540		1.539		1.539
ZT		0.566	↗	0.744	↗	**1**	↘	0.994	↘	**0.715**	↘	0.700
$(ZT)_{Mott}=\frac{\pi^2}{3\times\xi_p^2}$	↗	0.206		0.328		**0.9999**		1.166		3.290		3.421
Ts $\left(10^{-8}\frac{V}{K}\right)$		8788	↗	9637	↘	1.825	↘	−2056	↘	−16574	↘	−17070
Pt $(10^{-3}V)$		5.881	↗	8.089	↗	13.44	↗	14.02	↗	15.47	↘	15.43

In summary, from above Tables, for $\xi_{n(p)} \equiv \frac{\mathbb{E}_{Fn(Fp)}(N^*,T)}{k_B T} \gtrsim 1$, the maximal value of $\left|RD_{L,L_{VC}}\right|$ is equal to : 1.541×10^{-6}, suggesting that the above Wiedemann-Frank thermoelectric conversion law, ginen in Eq. (25a) is found to be exact, with the Laurenz 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 degenerate n(p)-type Si.

6. Concluding remarks

In the n(p)-type degenerate Si-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, $\varepsilon(r_{d(a)})$, 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:

(a) $\mathbb{E}_{Fno(Fpo)}(N^* = 0) = 0$, 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,

$\mathbb{E}_{gn1(gp1)}\left(N^* = 0, r_{d(a)}, T = 0\right) = \mathbb{E}_{gn2(gp2)}\left(N^* = 0, r_{d(a)}, T = 0\right) = \mathbb{E}_{Fgni(Fgpi)}\left(r_{d(a)}\right)$,

where $\mathbb{E}_{gn1(gp1)}$, $\mathbb{E}_{gn2(gp2)}$ and $\mathbb{E}_{Fgni(Fgpi)}$ 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 $\mathbb{E}^2_{Fno(Fpo)}$ or to $(N^*)^{4/3}$, giving rise to: $\sigma(N^* = 0, r_{d(a)}, T = 0) = 0$, and therefore, as discussed in Equations (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 $N^{EBT}_{CDn(CDp)}(r_{d(Ba)})$ are found to be equal to: $9.8(4.91) \times 10^{-6}$, 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 3, the numerical results of the OBG, given in Eq. (5), are obtained, suggesting that those are accurate to within 1.16%(2.68%), for P(B)-Si systems.

(3) In Table 5, those of the electrical conductivity, $\sigma(N^*, r_{d(a)}, T)$, given in Eq. (27), are obtained for the degenerate P-Si system, with an accuracy of the order of 7.5%, giving us confidence in the determination of other electrical-and-thermoelectric properties.

(4) In Tables 6 and 7, 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.

(5) In Tables 8 and 9, 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 $N(=10^{21}\ cm^{-3})$ is very high, N^* therefore decreases slowly, explaining the slow decrease (↘) in $\frac{\mathbb{E}_{Fn}(N^*,T=300K)}{k_B T}$, σ, κ, C_κ, and $\kappa_{App.}$, **(ii)** the numerical result: $\left|RD_{\kappa,\kappa_{App.}}\right|_{300K} \simeq 4.84 \times 10^{-3}$ confirms the $\kappa_{App.}$ -law, as that given in Eq. (25b), and finally, **(iii)** $\left|RD_{L,L_{VC}}\right| \simeq 1.535 \times 10^{-6}$ thus confirms in the degenerate Si-case the well-known Wiedemann-Frank, given in Eq. (25a), is found to be exact.

(6) Finally, in Tables 10 and 11, for a given N^* and for a given degenerate d(a)-Si 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: (↗, ↘). One notes here that with increasing T: **(i)** for $\xi_{n(p)} = 1.813$, while the values of Sb present a same minimum (maximum) $(Sb)_{min.(max.)}\left(= (\mp)1.563 \times 10^{-4}\frac{V}{K}\right)$, those of ZT show a same maximum $ZT_{max.}(= \mathbf{1})$, **(ii)** for $\xi_n = 1$, those of 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 $(ZT)_{Mott} = \frac{\pi^2}{3\times\xi^2_{n(p)}}$ present same results: $\simeq 1$ and 3.290, respectively, and finally, **(iv)** the maximal value of $\left|RD_{L,L_{VC}}\right|$ is approximately equal to 1.541×10^{-6}, suggesting that in the degenerate Si-case the Wiedemann-Frank, given in Eq. (25a), is exact.

(7) From above remarks **(5)** and **(6)**, given for the maximal values of $\left|RD_{L,L_{VC}}\right|$, being equal approximatively to 1.5×10^{-6}, 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 Si.

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 Si-crystals, the Fermi energy $\mathbb{E}_{Fn(Fp)} \equiv [\mathbb{E}_{fn} - \mathbb{E}_c]\left(\mathbb{E}_{Fp} \equiv \left[\mathbb{E}_v - \mathbb{E}_{fp}\right]\right)$, $\mathbb{E}_{c(v)}$ 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 phenomenon. It means that $N^* = 0$ at this transition.

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

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

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 Si is determined by :

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

where $F\left(N^*, r_{d(a)}, T\right) = au^{\frac{2}{3}}\left(1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}}\right)^{-\frac{2}{3}}$, 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:

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

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

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

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:

$$\frac{D\left(N^*, r_{d(a)}, T\right)}{\mu\left(N^*, r_{d(a)}, T\right)} \equiv \frac{N}{q} \times \frac{d\mathbb{E}_{Fn(Fp)}}{dN} \equiv \frac{k_B \times T}{q} \times \left(u\frac{d\theta_{n(p)}}{du}\right), \tag{A5}$$

where $\theta_n(u)$ 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

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

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 $u\to 0$, 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: $W^2\approx A^2u^{2B}$ and $u[V'\times W-V\times W']\approx\frac{2}{3}au^{2/3}A^2u^{2B}$, and therefore, in this highly degenerate case and at T=0K,

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

One notes that, for $N^*=0$, $\mathbb{E}_{Fno(Fpo)}(N^*)=0$, 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 $\mathbb{E}_{Fno(Fpo)}$ given in Eq. (A.7) by $\mathbb{E}_{Fn(Fp)}$ determined in Eq. (A.3), Eq. (A.7) thus becomes in the present degenerate case, as

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

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

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

$$r_{sn(sp)}(N^*,r_{d(a)})\equiv\left(\frac{3g_{c(v)}}{4\pi N^*}\right)^{1/3}\times\frac{1}{a_{Bn(Bp)}(r_{d(a)})}=1.1723\times10^8\times\left(\frac{g_{c(v)}}{N^*}\right)^{1/3}\times\frac{m^*_{n(p)}/m_o}{\varepsilon(r_{d(a)})}. \quad (B1)$$

Here, the values of $g_{c(v)}=3(2)$ and $(m^*_{n(p)}/m_o)$ are defined and given in Table 1.

In particular, in the following, $m^*_{n(p)}/m_o=m_r/m_o=0.1713$, is taken for evaluating the band gap narrowing (BGN), as used in Section 3. Therefore, the correlation energy of an effective electron gas, $\mathbb{E}_{CE}(r_{sn(sp)})$, is found to be given by [1]:

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

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

$$\Delta\mathbb{E}_{gn}(N^*,r_d)\simeq a_1\times\frac{\varepsilon_o}{\varepsilon(r_d)}\times N_r^{1/3}+a_2\times\frac{\varepsilon_o}{\varepsilon(r_d)}\times N_r^{\frac{1}{3}}\times(2.503\times[-\mathbb{E}_{CE}(r_{sn})\times r_{sn}])+a_3\times\left[\frac{\varepsilon_o}{\varepsilon(r_d)}\right]^{5/4}\times\sqrt{\frac{m_v}{m_r}}\times N_r^{1/4}+a_4\times\sqrt{\frac{\varepsilon_o}{\varepsilon(r_d)}}\times N_r^{1/2}\times 2+a_5\times\left[\frac{\varepsilon_o}{\varepsilon(r_d)}\right]^{\frac{3}{2}}\times N_r^{\frac{1}{6}},\ N_r\equiv\frac{N^*=N-N_{CDn}(r_d)}{9.999\times10^{17}cm^{-3}}, \quad (B3)$$

where $a_1=6.829\times10^{-3}(eV)$, $a_2=1.168\times10^{-3}(eV)$, $a_3=5.032\times10^{-3}(eV)$, $a_4=10.058\times10^{-3}(eV)$ and $a_5=1.455\times10^{-3}(eV)$, and

$$\Delta\mathbb{E}_{gp}(N^*,r_a)\simeq a_1\times\frac{\varepsilon_o}{\varepsilon(r_a)}\times N_r^{1/3}+a_2\times\frac{\varepsilon_o}{\varepsilon(r_a)}\times N_r^{\frac{1}{3}}\times\left(2.503\times[-\mathbb{E}_{CE}(r_{sp})\times r_{sp}]\right)+a_3\times\left[\frac{\varepsilon_o}{\varepsilon(r_a)}\right]^{5/4}\times\sqrt{\frac{m_c}{m_r}}\times N_r^{1/4}+2a_4\times\sqrt{\frac{\varepsilon_o}{\varepsilon(r_a)}}\times N_r^{1/2}+a_5\times\left[\frac{\varepsilon_o}{\varepsilon(r_a)}\right]^{\frac{3}{2}}\times N_r^{\frac{1}{6}},\ N_r\equiv\left(\frac{N^*=N-N_{CDp}(r_a)}{9.999\times10^{17}\ cm^{-3}}\right), \quad (B4)$$

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, $\Delta\mathbb{E}_{gn(gp)}(N^* = 0, r_a) = 0$, according to the MIT.

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