wjert, 2025, Vol. 11 Issue 6, 250-268. *Review Article* **ISSN 2454-695X**

World Journal of Engineering Research and Technology

WJERT

www.wjert.org **SJIF Impact Factor: 7.029**

NEW OPTICAL-AND-ELECTRICAL CONDUCTIVITY DUALITY AND ITS APPLICATIONS IN N(P)-TYPE DEGENERATE “COMPENSATED” A(1-X)B(X)-CRYSTALLINE ALLOY, ENHANCED BY OUR STATIC DIELECTRIC CONSTANT LAW, AND ACCURATE FERMI ENERGY (XX)

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Article Received on 25/04/2025 **Article Revised on 15/05/2025** **Article Accepted on 04/06/2025**

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ABSTRACT

In the $n^{+}(p^{+}) - A_{(1-x)}B_{x}$- crystalline alloy, $0 \leq x \leq 1$, x being the concentration, the optical coefficients, and the electrical-and-thermoelectric laws, relations, and various coefficients, being enhanced by : (i) our static dielectric constant law, $\varepsilon(r_{d(a)}, x)$, $r_{d(a)}$ being the donor (acceptor) d(a)-radius, given in Equations (1a, 1b), (ii) our accurate Fermi energy, $E_{Fn(Fp)}$, given in Eq. (11) and accurate with a precision of the order of 2.11×10^{-4} [9], affecting all the expressions of optical, and electrical-and-thermoelectric coefficients , (iii) our optical-and-electrical transformation duality given in Eq. (15), and finally (iv) our optical-and-electrical conductivity models, given in Eq. (18, 20), are now investigated, basing on our physical model, and Fermi-Dirac distribution function, as those given in our recent works.[1, 2] Then, some important remarks can be repoted as follows. (1) From Eq. (16), by basing on: $n(E, r_{d(a)})$ and $\sigma_{O}(N, r_{d(a)}, x, T, E)$, determined in Equations (17, 18), one obtains: (i) as $E = E_{gn1(gp1)}$, one gets: $\kappa(E) = 0$, $\varepsilon_{2}(E) = 0$, $\propto(E) = 0$, and $\sigma_{O}(E) = 0$, as those obtained in our previous work[2], and (ii) as $E \to \infty$, $n(E) \to$ constant, $\sigma_{O}(E) \to$ constant, $\propto(E) \to$ constant, $R(E) \to$ constant, $\kappa(E) \to 0$, $\varepsilon_{1}(E) \to$ constant, and $\varepsilon_{2}(E) \to 0$, as those obtained in our previous work.[2] (2) From Equations (20-26), for any given x, $r_{d(a)}$ and N (or T), with increasing T (or decreasing N), one obtains: (i) for $\xi_{n(p)} = \sqrt{\frac{\pi^2}{3}} \simeq 1.8138$, while the numerical results of the Seebeck coefficient S present a same minimum $(S)_{min.} \left(\simeq -1.563 \times 10^{-4} \frac{V}{K}\right)$, those of the figure of merit ZT show a same maxi**mum** $(ZT)_{max.} = 1$, (ii) for $\xi_{n(p)} = 1$, the numerical results of S, ZT, the Mott figure of merit $(ZT)_{Mott}$, the first Van-Cong coefficient VC1, and the Thomson coefficient Ts, present the same results: $-1.322 \times 10^{-4} \frac{V}{K}$, 0.715, 3.290, $1.105 \times 10^{-4} \frac{V}{K}$, and $1.657 \times 10^{-4} \frac{V}{K}$, respectively, and finally (iii) for $\xi_{n(p)} = \sqrt{\frac{\pi^2}{3}} \simeq 1.8138$, $(ZT)_{Mott} = 1$, as those given in our recent work.[1] It seems that these same results could represent **a new law in the thermoelectric properties, obtained in the degenerate case ($\xi_{n(p)} \geq 0$)**.

KEYWORDS: Optical-and-electrical conductivity, Seebeck coefficient (S), Figure of merit (ZT), First Van-Cong coefficient (VC1), Second Van-Cong coefficient (VC2), Thomson coefficient (Ts), Peltier coefficient (Pt).

INTRODUCTION

In the $\mathbf{n^+(p^+)} - A_{(1-x)}B_x$- crystalline alloy, $0 \leq x \leq 1$, x being the concentration, the optical coefficients, and the electrical-and-thermoelectric laws, relations, and various coefficients, being enhanced by :

(i) our static dielectric constant law, $\varepsilon(r_{d(a)}, x)$, $r_{d(a)}$ being the donor (acceptor) d(a)-radius, given in Equations (1a, 1b),

(ii) our accurate Fermi energy, $E_{Fn(Fp)}$, given in Eq. (11) and accurate with a precision of the order of 2.11×10^{-4} [9], affecting all the expressions of optical, and electrical-and-thermoelectric coefficients ,

(iii)our optical-and-electrical transformation duality given in Eq. (15), and finally

(iv)our optical-and-electrical conductivity models, given in Eq. (18, 20), are now investigated, basing on our physical model, and Fermi-Dirac distribution function, as those given in our recent works.[1, 2]

It should be noted here that for x=0, these obtained numerical results may be reduced to those given in the n(p)-type degenerate **A-crystal**.[3-13] Then, some important remarks can be repoted as follows.

(1) As observed in Equations (3, 5, 6), the critical impurity density $N_{CDn(CDp)}$, defined by the generalized Mott criterium in the metal-insulator transition (**MIT**), is just the density of electrons (holes), localized in the exponential conduction (valence)-band tail (**EBT**), $N^{EBT}_{CDn(CDp)}$, being obtained with a precision of the order of $\mathbf{3} \times \mathbf{10^{-7}}$, respectively, as given in our recent works.[3] Therefore, the effective electron (hole)-density can be defined as: $N^* \equiv N - N_{CDn(CDp)} \simeq N - N^{EBT}_{CDn(CDp)}$, N being the total impurity density, as that observed in the compensated crystals.

(2) The ratio of the inverse effective screening length $k_{sn(sp)}$ to Fermi wave number $k_{Fn(kp)}$ at 0 K, $R_{sn(sp)}(N^*)$, defined in Eq. (7), is valid at any N^*.

(3) One further notes that: (i) $\sigma_O(N, r_{d(a)}, x, T, E)$, given in Eq. (18), increases with increasing E for given $(N, r_{d(a)}, x, T$)-physical conditions, (ii) as $E = E_{gn1(gp1)}(N, r_{d(a)}, x, T)$, $\sigma_O(N, r_{d(a)}, x, T, E) = 0$, as investigated in our previous work [2], and (iii) as $E \to \infty$, the above result is reduced to the highest one, σ_{HO}, as given in Eq. (19).

(4) Further, from Eq. (16), by basing on: $n(E,\ r_{d(a)})$ and $\sigma_O(N, r_{d(a)}, x, T, E)$, determined in Equations (17, 18), one obtains: (i) as $E = E_{gn1(gp1)}$, one gets: $\kappa(E) = 0$, $\varepsilon_2(E) = 0$, $\propto (E) = 0$, and $\sigma_O(E) = 0$, as those obtained in our previous work[2], and (ii) as $E \to \infty$, $n(E) \to$ constant, $\sigma_O(E) \to$ constant, $\propto (E) \to$ constant, $R(E) \to$ constant, $\kappa(E) \to 0$, $\varepsilon_1(E) \to$ constant, and $\varepsilon_2(E) \to 0$, as those obtained in our previous work.[2]

(5) Finally, for any given x, $r_{d(a)}$ and N (or T), with increasing T (or decreasing N), one obtains: (i) for $\xi_{n(p)} = \sqrt{\frac{\pi^2}{3}} \simeq 1.8138$, while the numerical results of the Seebeck coefficient S present a same minimum $(S)_{min.}\left(\simeq -1.563 \times 10^{-4}\frac{V}{K}\right)$, those of the figure of merit ZT show a same maxi**mum** $(ZT)_{max.} = 1$, (ii) for $\xi_{n(p)} = 1$, the numerical results of S, ZT, the Mott figure of merit $(ZT)_{Mott}$, the first Van-Cong coefficient VC1, and the Thomson coefficient Ts, present the same results: $-1.322 \times 10^{-4}\frac{V}{K}$, 0.715, 3.290, $1.105 \times 10^{-4}\frac{V}{K}$, and $1.657 \times 10^{-4}\frac{V}{K}$, respectively, and finally (iii) for $\xi_{n(p)} = \sqrt{\frac{\pi^2}{3}} \simeq 1.8138$, $(ZT)_{Mott} = 1$, as those given in our recent work.[1] It seems that these same results could represent **a new law in the thermoelectric properties, obtained in the degenerate case ($\xi_{n(p)} \geq 0$).**

(6) Finally, our electrical-and-thermoelectric relation is given in Eq. (31) by: $\frac{k_B}{q} \times VC2\left(N, r_{d(a)}, x, T\right) \equiv -\frac{\partial s}{\partial \xi_{n(p)}} \times \frac{D\left(N, r_{d(a)}, x, T\right)}{\mu\left(N, r_{d(a)}, x, T\right)} \left(\frac{V^2}{K}\right)$, $\frac{k_B}{q} = \sqrt{\frac{3 \times L}{\pi^2}}$, according, in this work, to: $VC2\left(N, r_{d(a)}, x, T\right) \equiv -\frac{D\left(N, r_{d(a)}, x, T\right)}{\mu\left(N, r_{d(a)}, x, T\right)} \times 2 \times \frac{(ZT)_{Mott} \times [1-(ZT)_{Mott}]}{[1+(ZT)_{Mott}]^2}$ (V), being reduced to: $\frac{D}{\mu}$, VC1 and VC2, determined respectively in Equations (24, 27, 28). This can be **a new result**.

OUR STATIC DIELECTRIC CONSTANT LAW AND GENERALIZED MOTT CRITERIUM IN THE METAL-INSULATOR TRANSITION

First of all, in the $\mathbf{n^+(p^+)} - A_{(1-x)}B_x$- crystalline alloy at T=0 K[1, 2], we denote : the donor (acceptor) d(a)-radius by $r_{d(a)}$, the corresponding intrinsic one by: $\mathbf{r_{do(ao)}=r_A}$, the effective averaged numbers of equivalent conduction (valence)-bands by : $g_{c(v)}$, the unperturbed relative effective electron (hole) mass in conduction (valence) bands by: $m_{c(v)}(x)/m_o$, m_o being the free electron mass, the unperturbed relative static dielectric constant by: $\varepsilon_o(x)$, and the intrinsic band gap by: $E_{go}(x)$.

Therefore, we can define the effective donor (acceptor)-ionization energy in absolute values as: $E_{do(ao)}(x) = \frac{13600 \times [m_{c(v)}(x)/m_o]}{[\varepsilon_o(x)]^2}$ meV , and then, the isothermal bulk modulus, by : $B_{do(ao)}(x) \equiv \frac{E_{do(ao)}(x)}{\left(\frac{4\pi}{3}\right) \times \left(r_{do(ao)}\right)^3}$.

Our Static Dielectric Constant Law

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

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

Furthermore, we also showed that, as $r_{d(a)} > r_{do(ao)}$ ($r_{d(a)} < r_{do(ao)}$), the compression (dilatation) gives rise to the increase (the decrease) in the energy gap $E_{gn(gp)}(r_{d(a)}, x)$, and the effective donor (acceptor)-ionization energy $E_{d(a)}(r_{d(a)}, x)$ in absolute values, obtained in the effective Bohr model, which is represented respectively by : $\pm [\Delta\alpha(r_{d(a)}, x)]_{n(p)}$,

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

for $r_{d(a)} \geq r_{do(ao)}$, and for $r_{d(a)} \leq r_{do(ao)}$,

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

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

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

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

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

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

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

corresponding to the decrease in both $E_{gno(gpo)}(r_{d(a)}, x)$ and $E_{d(a)}(r_{d(a)}, x)$, with decreasing $r_{d(a)}$ and for a given x.

It should be noted that, in the following, all the electrical-and-thermoelectric properties strongly depend on this **new $\varepsilon(r_{d(a)}, x)$-law.**

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

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

Generalized Mott Criterium in the MIT

Now, it is interesting to remark that the critical total donor (acceptor)-density in the MIT at T=0 K, $N_{CDn(NDp)}(r_{d(a)},x)$, was given by the Mott's criterium, with an empirical parameter, $M_{n(p)}$, as[2, 3]:

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

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

This excellent one can be explained from the definition of the reduced effective Wigner-Seitz (**WS**) radius $r_{sn(sp),M}$, in the Mott's criterium, being characteristic of interactions, by :

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

being equal to, in particular, at N=$N_{CDn(CDp)}(r_{d(a)},x)$: $r_{sn(sp),M}\big(N_{CDn(CDp)}(r_{d(a)},x),r_{d(a)},x\big)$= **2.4813963**, for any $(r_{d(a)},x)$-values. Then, from Eq. (4), one also has:

$$N_{CDn(CDp)}(r_{d(a)},x)^{1/3}\times a_{Bn(Bp)}(r_{d(a)},x) = \left(\frac{3}{4\pi}\right)^{\frac{1}{3}}\times\frac{1}{2.4813963} = \mathbf{0.25} = \mathbf{(WS)}_{n(p)} = \mathbf{M}_{n(p)}, \tag{5}$$

explaining thus the existence of the Mott's criterium.

Furthermore, by using $M_{n(p)} = 0.25$, according to the empirical Heisenberg parameter $\boldsymbol{\mathcal{H}_{n(p)} = 0.47137}$, as those given in our previous work[3], we have also showed that $N_{CDn(CDp)}$ is just **the density of electrons (holes) localized in the exponential conduction (valence)-band tail**, $N^{EBT}_{CDn(CDp)}$, with a precision of the order of $\mathbf{2.82\ (2.88)\times 10^{-7}}$, respectively.[3]

It shoud be noted that the values of $M_{n(p)}$ and $\mathcal{H}_{n(p)}$ could be chosen so that those of $N_{CDn(CDp)}$ and $N^{EBT}_{CDn(CDp)}$ are found to be in good agreement with their experimental results.

Therefore, the density of electrons (holes) given in parabolic conduction (valence) bands can be defined, as that given in compensated materials:

$N^*(N,r_{d(a)},x) \equiv N - N_{CDn(NDp)}(r_{d(a)},x)$= N^*, for a presentation simplicity. (6)

In summary, as observed in Tables 7 and 8 of our previous paper[3], one remarks that, for a given x and an increasing $r_{d(a)}$, $\varepsilon(r_{d(a)},x)$ decreases, while $E_{gno(gpo)}(r_{d(a)},x)$,

$N_{CDn(NDp)}(r_{d(a)}, x)$ and $N^{EBT}_{CDn(CDp)}(r_{d(a)}, x)$ increase, affecting strongly all electrical-and-thermoelectric properties, as those observed in following Sections.

PHYSICAL MODEL

In the $n^{+}(p^{+}) - A_{(1-x)}B_x$- crystalline alloy, the reduced effective Wigner-Seitz (**WS**) radius $r_{sn(sp)}$, characteristic of interactions, being given in Eq. (4), in which N is replaced by N^*, is now defined by:

$\gamma \times r_{sn(sp)}(N^*) \equiv \frac{k^{-1}_{Fn(Fp)}}{\alpha_{Bn(Bp)}} < 1$, $r_{sn(sp)}(N, r_{d(a)}, x) \equiv \left(\frac{3g_{c(v)}}{4\pi N^*}\right)^{1/3} \times \frac{1}{a_{Bn(Bp)}(r_{d(a)}, x)}$, 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 $a_{Bn(Bp)}(r_{d(a)}, x)$ is determined in Eq. (2).

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

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

being valid at any N^*.

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

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

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

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

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

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

Where $E_{CE}(N^*)$ is the majority-carrier correlation energy (CE), being determined by:

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

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

$$\frac{k_{Fn(Fp)}^{-1}}{a_{Bn(Bp)}} < \frac{\eta_{n(p)}}{E_{Fno(Fpo)}} \equiv \frac{1}{A_{n(p)}} < \frac{k_{Fn(Fp)}^{-1}}{k_{sn(sp)}^{-1}} \equiv R_{sn(sp)} < 1, \ \eta_{n(p)}(N^*) \equiv \frac{\sqrt{2\pi \times (\frac{N^*}{g_{c(v)}})}}{\varepsilon(r_{d(a)})} \times q^2 k_{sn(sp)}^{-1/2}, \qquad (9b)$$

Which gives: $A_{n(p)}(N^*) = \frac{E_{Fno(Fpo)}(N^*)}{\eta_{n(p)}(N^*)}$, $E_{Fno(Fpo)}(N^*) \equiv \frac{\hbar^2 \times k_{Fn(Fp)}^2(N^*)}{2 \times m_{c(v)}(x) \times m_o}$.

BAND GAP NARROWING (BGN) BY N AND BY T

First, the BGN by N is found to be given by[2]

$$\Delta E_{gn(gp);N}(N^*, r_{d(a)}, x) \simeq a_1 + \frac{\varepsilon_o(x)}{\varepsilon(r_{d(a)}, x)} \times N_r^{\frac{1}{3}} + a_2 \times \frac{\varepsilon_o(x)}{\varepsilon(r_{d(a)}, x)} \times N_r^{\frac{1}{3}} \times \left(2.503 \times [-E_{CE}(r_{sn(sp)})] \times r_{sn(sp)}\right) + a_3 \times \left[\frac{\varepsilon_o(x)}{\varepsilon(r_{d(a)}, x)}\right]^{\frac{5}{4}} \times \sqrt{\frac{m_p}{m_r}} \times N_r^{\frac{1}{4}} + 2a_4 \times \left[\frac{\varepsilon_o(x)}{\varepsilon(r_{d(a)}, x)}\right]^{\frac{1}{2}} \times N_r^{\frac{1}{2}} + 2a_5 \times \left[\frac{\varepsilon_o(x)}{\varepsilon(r_{d(a)}, x)}\right]^{\frac{3}{2}} \times N_r^{\frac{1}{6}}, \ N_r = \frac{N^*}{9.999 \times 10^{17}\ \text{cm}^{-3}}, \qquad (10a)$$

Here, $a_1 = 3.8 \times 10^{-3}\,(\text{eV})$, $a_2 = 6.5 \times 10^{-4}\,(\text{eV})$, $a_3 = 2.85 \times 10^{-3}\,(\text{eV})$, $a_4 = 5.597 \times 10^{-3}\,(\text{eV})$, and $a_5 = 8.1 \times 10^{-4}\,(\text{eV})$.

Therefore, at T=0 K and $N^* = 0$, and for any $r_{d(a)}$, one gets: $\Delta E_{gn(gp)} = 0$, according to the metal-insulator transition (MIT).

Secondly, one has[2]:

$$\Delta E_{gn(gp);T}(T) = 0.20251 \times \left(\left[1 + \left(\frac{2T}{440.0613\ K}\right)^{2.201}\right]^{\frac{1}{2.201}} - 1\right). \qquad (10b)$$

FERMI ENERGY AND FERMI-DIRAC DISTRIBUTION FUNCTION

Fermi Energy

Here, for a presentation simplicity, we change all the sign of various parameters, given in the $p^+ - A_{(1-x)}B_x$ - crystalline alloy in order to obtain the same one, as given in the $n^+ - A_{(1-x)}B_x$ - crystalline alloy, according to the reduced Fermi energy $E_{Fn(Fp)}$, $\xi_{n(p)}(N, r_{d(a)}, x, T) \equiv \frac{E_{Fn(Fp)}(N, r_{d(a)}, x, T)}{k_B T} > 0 (< 0)$, obtained respectively in the degenerate (non-degenerate) case.

For any $(N, r_{d(a)}, x, T)$, the reduced Fermi energy $\xi_{n(p)}(N, r_{d(a)}, x, T)$ or the Fermi energy $E_{Fn(Fp)}(N, r_{d(a)}, x, T)$, obtained in our previous paper[9], obtained with a precision of the order of 2.11×10^{-4}, is found to be given by:

$$\xi_{n(p)}(u) \equiv \frac{E_{Fn(Fp)}(u)}{k_B T} = \frac{G(u) + Au^B F(u)}{1 + Au^B} \equiv \frac{V(u)}{W(u)}, \ A = 0.0005372 \text{ and } B = 4.82842262, \qquad (11)$$

Where u is the reduced electron density, $u(N, r_{d(a)}, x, T) \equiv \frac{N^*}{N_{c(v)}(T,x)}$, $N_{c(v)}(T,x) = 2g_{c(v)} \times \left(\frac{m_{c(v)}(x) \times m_o \times k_B T}{2\pi\hbar^2}\right)^{\frac{3}{2}}$ (cm^{-3}), $F(u) = au^{\frac{2}{3}}\left(1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}}\right)^{-\frac{2}{3}}$, $a = [3\sqrt{\pi}/4]^{2/3}$, $b = \frac{1}{8}\left(\frac{\pi}{3}\right)^2$, $c = \frac{62.3739855}{1920}\left(\frac{\pi}{3}\right)^4$, and $G(u) \simeq Ln(u) + 2^{-\frac{3}{2}} \times u \times e^{-du}$; $d = 2^{3/2}\left[\frac{1}{\sqrt{27}} - \frac{3}{16}\right] > 0$.

So, in the non-degenerate case $(u \ll 1)$, one has: $E_{Fn(Fp)}(u) = k_B T \times G(u) \simeq k_B T \times Ln(u)$ as **$u \longrightarrow 0$, the limiting non-degenerate condition**, and in the very degenerate case $(u \gg 1)$, one gets: $E_{Fn(Fp)}(u \gg 1) = k_B T \times F(u) = k_B T \times au^{\frac{2}{3}}\left(1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}}\right)^{-\frac{2}{3}} \simeq \frac{\hbar^2 \times k_{Fn(Fp)}^2(N^*)}{2 \times m_{c(v)}(x) \times m_o}$ as **$u \longrightarrow \infty$, the limiting degenerate condition**. In other words, $\xi_{n(p)} \equiv \frac{E_{Fn(Fp)}}{k_B T}$ is accurate, and it also verifies the correct limiting conditions.

In particular, at T=0K, since $u^{-1} = 0$, Eq. (11) is reduced to: $E_{Fno(Fpo)}(N^*) \equiv \frac{\hbar^2 \times k_{Fn(Fp)}^2(N^*)}{2 \times m_{c(v)}(x) \times m_o}$, being proportional to $(N^*)^{2/3}$, and also equal to 0 at $N^* = 0$, according to the MIT.

In the following, it should be noted that all the electrical-and-thermoelectric properties strongly depend on such the accurate expression of $\xi_{n(p)}(N, r_{d(a)}, x, T)$.[9]

Fermi-Dirac Distribution Function (FDDF)

The Fermi-Dirac distribution function (FDDF) is given by: $f(E) \equiv (1 + e^{\gamma})^{-1}$, $\gamma \equiv (E - E_{Fn(Fp)})/(k_B T)$.

So, the average of E^p, calculated using the FDDF-method, as developed in our previous works[1, 6] is found to be given by:

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

Further, one notes that, at 0 K, $-\frac{\partial f}{\partial E} = \delta(E - E_{Fno(Fpo)})$, $\delta(E - E_{Fno(Fpo)})$ being the Dirac delta (δ)-function. Therefore, $G_p(E_{Fno(Fpo)}) = 1$.

Then, at low T, by a variable change $\gamma \equiv (E - E_{Fn(Fp)})/(k_B T)$, one has:

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

Where $C_p^\beta \equiv p(p-1)\ldots(p-\beta+1)/\beta!$ 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:

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

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 above Eq. of $\langle E^p \rangle_{FDDF}$, we get in the degenerate case the following ratio:

$$G_p\left(E_{Fn(Fp)}\right) \equiv \frac{\langle E^p \rangle_{FDDF}}{E_{Fn(Fp)}^p} = 1 + \sum_{n=1}^{p} \frac{p(p-1)\ldots(p-2n+1)}{(2n)!} \times (2^{2n}-2) \times |B_{2n}| \times y^{2n} \equiv G_{p\geq 1}(y), \quad (12)$$

Where $y \equiv \frac{\pi}{\xi_{n(p)}(N^*,T)} = \frac{\pi k_B T}{E_{Fn(Fp)}(N^*,T)}$.

Then, some usual results of $G_{p\geq 1}(y)$ are given in Table 2 in Appendix 1, being needed to determine all the following electrical-and-thermoelectric properties.

Table 1: Expressions for $G_{p\geq 1}(y \equiv \frac{\pi}{\xi_{n(p)}})$, due to the Fermi-Dirac distribution function, noting that $G_{p=1}(y \equiv \frac{\pi k_B T}{E_{Fn(Fp)}} = \frac{\pi}{\xi_{n(p)}}) = 1$, used to determine the electrical-and-thermoelectric coefficients.

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

OPTICAL-AND-ELECTRICAL PROPERTIES

Optical-and-Electrical Transformation Duality

First off on, for a presentation simplicity, we change all the sign of various parameters, given in the $p^+ - A_{(1-x)}B_x$-crystalline alloy, in order to obtain the same one, as given in the $n^+ - A_{(1-x)}B_x$ - crystalline alloy, according to the reduced Fermi energy $E_{Fn(Fp)}$, $\xi_{n(p)}(N, r_{d(a)}, x, T) \equiv \frac{E_{Fn(Fp)}(N, r_{d(a)}, x, T)}{k_B T} > 0(< 0)$, obtained respectively in the degenerate (non-degenerate) case, giving: $E_{Fno(Fpo)} \equiv E_{Fn(Fp)}(N, r_{d(a)}, x, T = 0)$.

Then, in the $n^{+}(p^{+}) - A_{(1-x)}B_{x}$- degenerate crystalline alloy and for the temperature T(K), if denoting:

(i) for the electrical phenomenon (EP), the effective mass by $m^{*}_{n(p)}/m_{o}$, m_{o} being the free electron mass, is equal respectively to: the electron (hole) mass, $m_{c(v)}/m_{o}$, given in the conduction (valence)-band, corresponding the reduced band gap, defined by:

$$E_{gn2(gp2)} \equiv E_{c(v)} - E_{vo(co)} = E_{gni(gpi)} - \Delta E_{gn(gp);N}(N^{*}) - \Delta E_{gn(gp);T}(T), \tag{13}$$

where $E_{gni(gpi)}$ is the intrinsic bang gap, $\Delta E_{gn(gp)}(N^{*})$ and $\Delta E_{gn(gp)}(T)$ are respectively the reduced band gaps, due to the N^{*}-and-T effects, as those determined in our previous work[2], and (ii) for the optical phenomenon (OP), $E \equiv \hbar\omega$ is the photon energy, the effective mass by $m^{*}_{n(p)}/m_{o}$ is equal to: the reduced (or relative) mass, $m_{r}/m_{o} \equiv m_{r}/m_{o} \equiv \frac{m_{c}\times m_{v}}{m_{c}+m_{v}}$, corresponding the optical band gap, $E_{gn1(gp1)}$, defined by: $E_{gn1(gp1)} \equiv E_{gn2(gp2)} + E_{Fn(Fp)}$; therefore, for $E \geq E_{gn1(gp1)}$, one has:

$$E - E_{gn1(gp1)} = E - \left(E_{gn2(gp2)} + E_{Fn(Fp)}\right). \tag{14}$$

From above Equations, one uses an optical-and-electrical transformation duality, as:

$E - E_{gn1(gp1)} \geq 0$, for the OP, is reduced, as $E = E_{gn1(gp1)} + E_{Fn(Fp)}\left[E_{Fno(Fpo)}\right]$, for the EP, to: $E - E_{gn1(gp1)} = E_{Fn(Fp)}\left[E_{Fno(Fpo)}\right]$, and reciprocally. (15)

Eq. (15) shows that, for both EP and OP, the Fermi energy-level penetrations into conduction (valence)-bands, observed in the $n^{+}(p^{+}) -$ type degenerate $A_{(1-x)}B_{x}$ -crystalline alloy, $E_{Fn(Fp)}\left[E_{Fno(Fpo)}\right]$, are well defined.

Furthermore, for the OP, if denoting wave number by k, the kinetic energy E_{k} is given by: $E_{k} \equiv \frac{\hbar^{2}\times k^{2}}{2\times m_{r}(x)\times m_{o}}$ and the Fermi energy $E_{Fn(Fp)}$ by: $E_{gn1(gp1)} - E_{gn2(gp2)} \equiv E_{Fn(Fp)} = \frac{\hbar^{2}\times k^{2}_{Fn(Fp)}}{2\times m^{*}_{n(p)}\times m_{o}}$, $k_{Fn(Fp)}$ being the Fermi wave: $k_{Fn(Fp)}(N^{*}) \equiv \left(\frac{3\pi^{2}N^{*}}{g_{c(v)}}\right)^{\frac{1}{3}}$, where $g_{c(v)}$ is the effective averaged numbers of equivalent conduction (valence)-bands.

Optical Coefficients

The optical properties for any medium can be described by the complex refraction: $\mathbb{N} \equiv n - i\kappa$, n and κ being the refraction index and the extinction coefficient, the complex dielectric function: $\mathcal{E} = \varepsilon_{1} - i\varepsilon_{2}$, where $i^{2} = -1$, and $\mathcal{E} = \mathbb{N}^{2}$. Further, if denoting the normal-incidence reflectance and the optical absorption by R and $\propto$, one gets:

$$\propto (E) = \frac{E \times \varepsilon_2(E)}{\hbar c n(E)} = \frac{2E \times \kappa(E)}{\hbar c} = \frac{4\pi \sigma_O(E)}{cn(E) \times \varepsilon_{\text{free space}}},\ \varepsilon_1 \equiv n^2 - \kappa^2, \varepsilon_2 \equiv 2\kappa n, \text{ and } R(E) \equiv \frac{[n-1]^2+\kappa^2}{[n+1]^2+\kappa^2}, \quad (16)$$

Where the refraction index n is found to be defined by :

$$n(E,\ r_{d(a)}) \equiv n_\infty(r_{d(a)}) + \sum_{i=1}^{4} \frac{B_{0i}E + C_{0i}}{E^2 - B_1E + C_i} \to n_\infty\left(r_{d(a)}\right) \text{ as } E \to \infty. \quad (17)$$

Here, the optical conductivity σ_O can be defined and expressed in terms of the kinetic energy of the electron (hole), $E_k \equiv \frac{\hbar^2 \times k^2}{2 \times m_{c(v)}(x) \times m_o}$, or the wave number k, as:

$$\sigma_O(k) \equiv \frac{q^2 \times k}{\pi \times \hbar} \times \frac{k}{k_{sn(sp)}} \times \left[k \times a_{Bn(Bp)}\right] \times \left(\frac{E_k}{\eta_{n(p)}}\right)^{1/2},$$

Which is thus proportional to $E_k{}^2$.

Then, we obtain $\langle E^2 \rangle_{FDDF} \equiv G_2(y = \frac{\pi k_B T}{E_{Fn(Fp)}}) \times E^2_{Fn(Fp)}$, and $G_2(y) = \left(1 + \frac{y^2}{3}\right) \equiv G_2(N, r_{d(a)}, x, T)$, with $y \equiv \frac{\pi}{\xi_{n(p)}}$, $\xi_{n(p)} = \xi_{n(p)}\left(N, r_{d(a)}, x, T\right)$ for a presentation simplicity. Therefore, one obtains[1]:

$$\sigma_O\left(N, r_{d(a)}, x, T, E\right) = \left[\frac{q^2}{\pi \times \hbar} \times \frac{k_{Fn(Fp)}(N^*)}{R_{sn(sp)}(N^*)} \times \left[k_{Fn(Fp)}(N^*) \times a_{Bn(Bp)}\left(r_{d(a)}\right)\right] \times \sqrt{A_{n(p)}(N^*)}\right] \times G_2\left(N, r_{d(a)}, x, T\right) \times \left[\left(\frac{E - E_{gn1(gp1)}\left(N, r_{d(a)}, x, T\right)}{E - E_{gn1(gp1)}\left(N, r_{d(a)}, x, T=0\right)}\right)^2\right] \left(\frac{1}{\text{ohm} \times \text{cm}}\right), \quad (18)$$

Where $E - E_{gn1(gp1)} \equiv E - E_{gn2(gp2)} - E_{Fn(Fp)} \geq 0$, $\frac{q^2}{\pi \times \hbar} = 7.7480735 \times 10^{-5}\ \text{ohm}^{-1}$, $A_{n(p)}(N^*) = \frac{E_{Fno(Fpo)}(N^*)}{\eta_{n(p)}(N^*)}$, $R_{sn(sp)}(N^*) \equiv \frac{k_{sn(sp)}}{k_{Fn(Fp)}}$. This result should be new in comparison with that, obtained from an improved Forouhi-Bloomer parameterization, as given in our previous work.[2]

Consequently, from Eq. (16), by basing on: $n(E,\ r_{d(a)})$ and $\sigma_O\left(N, r_{d(a)}, x, T, E\right)$, determined in Equations (17, 18), one obtains:

(i) as $E = E_{gn1(gp1)}$, one gets: $\kappa(E) = 0$, $\varepsilon_2(E) = 0$, $\propto (E) = 0$, and $\sigma_O(E) = 0$, as those obtained in our previous work[2], and

(ii) as $E \to \infty$, $n(E) \to$ constant, $\sigma_O(E) \to$ constant, $\propto (E) \to$ constant, $R(E) \to$ constant, $\kappa(E) \to 0$, $\varepsilon_1(E) \to$ constant, and $\varepsilon_2(E) \to 0$, as those obtained in our previous work.[2]

One further notes that: (i) $\sigma_O\left(N, r_{d(a)}, x, T, E\right)$ increases with increasing E for given $(N, r_{d(a)}, x, T)$-physical conditions, (ii) as $E = E_{gn1(gp1)}\left(N, r_{d(a)}, x, T\right)$, $\sigma_O\left(N, r_{d(a)}, x, T, E\right) = 0$, as investigated in our previous work[2], and (iii) as $E \rightarrow \infty$, the above result is reduced to the highest one, σ_{HO}, as:

$$\sigma_{HO}\left(N, r_{d(a)}, x, T, E\right) = \left[\frac{q^2}{\pi \times \hbar} \times \frac{k_{Fn(Fp)}(N^*)}{R_{sn(sp)}(N^*)} \times \left[k_{Fn(Fp)}(N^*) \times a_{Bn(Bp)}\left(r_{d(a)}\right)\right] \times \sqrt{A_{n(p)}(N^*)}\right] \times G_2\left(N, r_{d(a)}, x, T\right). \qquad (19)$$

Now, using the optical-and-electrical transformation duality (15), one obtains the electrical conductivity, σ, defined by:

$$\sigma\left(N, r_{d(a)}, x, T\right) = \left[\frac{q^2}{\pi \times \hbar} \times \frac{k_{Fn(Fp)}(N^*)}{R_{sn(sp)}(N^*)} \times \left[k_{Fn(Fp)}(N^*) \times a_{Bn(Bp)}\left(r_{d(a)}\right)\right] \times \sqrt{A_{n(p)}(N^*)}\right] \times \left[G_2\left(N, r_{d(a)}, x, T\right) \times \left(\frac{E_{Fn(Fp)}\left(N, r_{d(a)}, x, T\right)}{E_{Fno(Fpo)}\left(N, r_{d(a)}, x, T=0\right)}\right)^2\right] \left(\frac{1}{ohm \times cm}\right), \qquad (20)$$

as that investigated in our recent work.[1]

ELECTRICAL-AND-THERMOELECTRIC PROPERTIES

Here, if denoting, for majority electrons (holes), the electrical conductivity by $\sigma(N, r_{d(a)}, x, T)$ expressed in $ohm^{-1} \times cm^{-1}$, the thermal conductivity by $\sigma_T(N, r_{d(a)}, x, T)$ in $\frac{W}{cm \times K}$, and the Lorenz number L defined by: $L = \frac{\pi^2}{3} \times \left(\frac{k_B}{q}\right)^2 = 2.4429637 \left(\frac{W \times ohm}{K^2}\right) = 2.4429637 \times 10^{-8} \, (V^2 \times K^{-2})$, then the well-known Wiedemann-Frank law states that the ratio, $\frac{\kappa}{\sigma}$, is proportional to the temperature T(K), as:

$$\frac{\sigma_T(N, r_{d(a)}, x, T)}{\sigma(N, r_{d(a)}, x, T)} = L \times T. \qquad (21)$$

We now determine the general form of σ in the following.

Which can be used to define the resistivity as: $\rho(N, r_{d(a)}, x, T) \equiv 1/\sigma(N, r_{d(a)}, x, T)$, noting again that $N^* \equiv N - N_{CDn(NDp)}(r_{d(a)}, x)$. This $\sigma\left(N, r_{d(a)}, x, T\right)$-result is an essential one in this paper, being used to determine other electrical-and-thermoelectric properties.

In Eq. (20), one notes that at T= 0 K, $\sigma(N, r_{d(a)}, x, T = 0K)$ is proportional to $E^2_{Fno(Fpo)}$, or to $(N^*)^{\frac{4}{3}}$. Thus, $\sigma(N = N_{CDn(NDp)}, r_{d(a)}, x, T = 0K) = 0$ at $N^* = 0$, at which the MIT occurs.

Electrical Coefficients

The relaxation time τ is related to σ by[1]:

$\tau(N, r_{d(a)}, x, T) \equiv \sigma(N, r_{d(a)}, x, T) \times \frac{m_{c(v)}(x) \times m_o}{q^2 \times (N^*/g_{c(v)})}$. Therefore, the mobility μ is given by:

$$\mu\left(N, r_{d(a)}, x, T\right) \equiv \mu\left(N^{*}, r_{d(a)}, T\right) = \frac{q\times\tau\left(N, r_{d(a)}, x, T\right)}{m_{c(v)}(x)\times m_{o}} = \frac{\sigma\left(N, r_{d(a)}, x, T\right)}{q\times(N^{*}/g_{c(v)})}\ \left(\frac{cm^{2}}{V\times s}\right). \quad (22)$$

Here, at T= 0K, $\mu(N^{*}, r_{d(a)}, T)$ 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 MIT occurs.

Then, since τ and σ are both proportional to $E_{Fn(Fp)}(N^{*}, T)^{2}$, as given above, the Hall factor is defined by:

$r_{H}(N, r_{d(a)}, x, T) \equiv \frac{(\tau^{2})_{FDDF}}{[(\tau)_{FDDF}]^{2}} = \frac{G_{4}(y)}{[G_{2}(y)]^{2}}$, $y \equiv \frac{\pi}{\xi_{n(p)}(N, r_{d(a)}, x, T)} = \frac{\pi k_{B}T}{E_{Fn(Fp)}(N, r_{d(a)}, x, T)}$, and therefore, the Hall mobility yields:

$$\mu_{H}\left(N, r_{d(a)}, x, T\right) \equiv \mu\left(N, r_{d(a)}, x, T\right) \times r_{H}(N^{*}, T)\ \left(\frac{cm^{2}}{V\times s}\right), \quad (23)$$

Noting that, at T=0K, since $r_{H}(N, r_{d(a)}, x, T) = 1$, one then gets: $\mu_{H}(N, r_{d(a)}, x, T) \equiv \mu(N, r_{d(a)}, x, T)$.

Our generalized Einstein relation

Our generalized Einstein relation is found to be defined as[1]:

$$\frac{D\left(N, r_{d(a)}, x, T\right)}{\mu\left(N, r_{d(a)}, x, T\right)} \equiv \frac{N^{*}}{q}\times\frac{dE_{Fn(Fp)}}{dN^{*}} \equiv \frac{k_{B}\times T}{q}\times\left(u\frac{d\xi_{n(p)}(u)}{du}\right) = \sqrt{\frac{3\times L}{\pi^{2}}}\times T\times\left(u\frac{d\xi_{n(p)}(u)}{du}\right),\ \frac{k_{B}}{q} = \sqrt{\frac{3\times L}{\pi^{2}}} \quad (24)$$

Where $D\left(N, r_{d(a)}, x, T\right)$ is the diffusion coefficient, $\xi_{n(p)}(u)$ is defined in Eq. (11), and the mobility $\mu\left(N, r_{d(a)}, x, T\right)$ is determined in Eq. (22). Then, by differentiating this function $\xi_{n(p)}(u)$ with respect to u, one thus obtains $\frac{d\xi_{n(p)}(u)}{du}$. Therefore, Eq. (17) can also be rewritten as:

$$\frac{D\left(N, r_{d(a)}, x, T\right)}{\mu\left(N, r_{d(a)}, x, T\right)} = \frac{k_{B}\times T}{q}\times u\,\frac{V'(u)\times W(u) - V(u)\times W'(u)}{W^{2}(u)},$$

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 $u[V' \times W - V \times W'] \approx \frac{2}{3}au^{2/3}A^{2}u^{2B}$, and therefore, in this **highly degenerate case** and at T=0K, the **above generalized Einstein relation** is reduced to the **usual Einstein one**:

$\frac{D(N, r_{d(a)}, x, T=0\ K)}{\mu(N, r_{d(a)}, x, T=0\ K)} \approx \frac{2}{3} E_{Fno(Fpo)}(N^*)/q$. In other words, **Eq. (24) verifies the correct limiting conditions**.

Furthermore, in the present degenerate case ($u \gg 1$), Eq. (24) gives:

$$\frac{D(N, r_{d(a)}, x, T)}{\mu(N, r_{d(a)}, x, T)} \simeq \frac{2}{3} \times \frac{E_{Fno(Fpo)}(u)}{q} \times \left[1 + \frac{4}{3} \times \frac{\left(bu^{-\frac{4}{3}} + 2cu^{-\frac{8}{3}}\right)}{\left(1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}}\right)}\right],$$

Where $a = [3\sqrt{\pi}/4]^{2/3}$, $b = \frac{1}{8}\left(\frac{\pi}{3}\right)^2$ and $c = \frac{62.3739855}{1920}\left(\frac{\pi}{3}\right)^4$.

Thermoelectric Coefficients

First of all, from Eq. (20), obtained for $\sigma(N, r_{d(a)}, x, T)$, the well-known Mott definition for the thermoelectric power or for the Seebeck coefficient, S, is found to be given by:

$$S(N, r_{d(a)}, x, T) \equiv \frac{-\pi^2}{3} \times \frac{k_B}{q>0} \times k_B T \times \left.\frac{\partial \ln \sigma(E)}{\partial E}\right]_{E=E_{Fn(Fp)}} = \frac{-\pi^2}{3} \times \frac{k_B}{q} \times \frac{\partial \ln \sigma(\xi_{n(p)})}{\partial \xi_{n(p)}}.$$

Then, using Eq. (11), for the degenerate case, $\xi_{n(p)} \geq 0$, one gets, by putting $F_S(N, r_{d(a)}, x, T) \equiv \left[1 - \frac{y^2}{3 \times G_2\left(y = \frac{\pi}{\xi_{n(p)}}\right)}\right]$,

$$S(N, r_{d(a)}, x, T) \equiv \frac{-\pi^2}{3} \times \frac{k_B}{q} \times \frac{2F_{Sb}(N^*, T)}{\xi_{n(p)}} = -\sqrt{\frac{3 \times L}{\pi^2}} \times \frac{2 \times \xi_{n(p)}}{\left(1 + \frac{3 \times \xi_{n(p)}^2}{\pi^2}\right)} = -2\sqrt{L} \times \frac{\sqrt{(ZT)_{Mott}}}{1 + (ZT)_{Mott}}\left(\frac{V}{K}\right) < 0, \quad (ZT)_{Mott} = \frac{\pi^2}{3 \times \xi_{n(p)}^2}, \quad (25)$$

according to:

$$\frac{\partial S}{\partial \xi_{n(p)}} = \sqrt{\frac{3 \times L}{\pi^2}} \times 2 \times \frac{\frac{3 \times \xi_{n(p)}^2}{\pi^2} - 1}{\left(1 + \frac{3 \times \xi_{n(p)}^2}{\pi^2}\right)^2} = \sqrt{\frac{3 \times L}{\pi^2}} \times 2 \times \frac{(ZT)_{Mott} \times [1 - (ZT)_{Mott}]}{[1 + (ZT)_{Mott}]^2}.$$

Here, one notes that: (i) as $\xi_{n(p)} \to +\infty$ or $\xi_{n(p)} \to +0$, one has a same limiting value of S: $S \to -0$, (ii) at $\xi_{n(p)} = \sqrt{\frac{\pi^2}{3}} \simeq 1.8138$, since $\frac{\partial S}{\partial \xi_{n(p)}} = 0$, one therefore gets: a minimum $(S)_{min.} = -\sqrt{L} \simeq -1.563 \times 10^{-4} \left(\frac{V}{K}\right)$, and (iii) at $\xi_{n(p)} = 1$ one obtains: $S \simeq -1.322 \times 10^{-4} \left(\frac{V}{K}\right)$.

Further, the figure of merit, ZT, is found to be defined by:

$$\mathrm{ZT}(\mathrm{N}, \mathrm{r}_{\mathrm{d(a)}}, \mathrm{x}, \mathrm{T}) \equiv \frac{\mathrm{S}^2 \times \sigma \times \mathrm{T}}{\kappa} = \frac{\mathrm{S}^2}{\mathrm{L}} = \frac{4 \times (\mathrm{ZT})_{\mathrm{Mott}}}{[1+(\mathrm{ZT})_{\mathrm{Mott}}]^2}. \tag{26}$$

Here, one notes that: (i) $\frac{\partial(\mathrm{ZT})}{\partial \xi_{\mathrm{n(p)}}} = 2 \times \frac{\mathrm{S}}{\mathrm{L}} \times \frac{\partial \mathrm{S}}{\partial \xi_{\mathrm{n(p)}}}$, $\mathrm{S} < 0$, (ii) at $\xi_{\mathrm{n(p)}} = \sqrt{\frac{\pi^2}{3}} \simeq 1.8138$, since $\frac{\partial(\mathrm{ZT})}{\partial \xi_{\mathrm{n(p)}}} = 0$, one gets: a maximum $(\mathrm{ZT})_{\mathrm{max.}} = 1$,and $(\mathrm{ZT})_{\mathrm{Mott}} = 1$, and (iii) at $\xi_{\mathrm{n(p)}} = 1$, one obtains: $\mathrm{ZT} \simeq 0.715$ and $(\mathrm{ZT})_{\mathrm{Mott}} = \frac{\pi^2}{3} \simeq 3.290$.

Finally, the first Van-Cong coefficient, VC1, can be defined by:

$$\mathrm{VC1}(\mathrm{N}, \mathrm{r}_{\mathrm{d(a)}}, \mathrm{x}, \mathrm{T}) \equiv -\mathrm{N}^* \times \frac{\mathrm{dS}}{\mathrm{dN}^*} \left(\frac{\mathrm{V}}{\mathrm{K}}\right) = \mathrm{N}^* \times \frac{\partial S}{\partial \xi_{\mathrm{n(p)}}} \times -\frac{\partial \xi_{\mathrm{n(p)}}}{\partial \mathrm{N}^*}, \text{ being equal to 0 for } \xi_{\mathrm{n(p)}} = \sqrt{\frac{\pi^2}{3}}, \tag{27}$$

And the second Van-Cong coefficient, $\mathrm{VC2}$, as:

$$\mathrm{VC2}(\mathrm{N}, \mathrm{r}_{\mathrm{d(a)}}, \mathrm{x}, \mathrm{T}) \equiv \mathrm{T} \times \mathrm{VC1}\ (\mathrm{V}), \tag{28}$$

The Thomson coefficient, Ts, by:

$$\mathrm{Ts}(\mathrm{N}, \mathrm{r}_{\mathrm{d(a)}}, \mathrm{x}, \mathrm{T}) \equiv \mathrm{T} \times \frac{\mathrm{dS}}{\mathrm{dT}} \left(\frac{\mathrm{V}}{\mathrm{K}}\right) = \mathrm{T} \times \frac{\partial S}{\partial \xi_{\mathrm{n(p)}}} \times \frac{\partial \xi_{\mathrm{n(p)}}}{\partial \mathrm{T}}, \text{ being equal to 0 for } \xi_{\mathrm{n(p)}} = \sqrt{\frac{\pi^2}{3}}, \tag{29}$$

and the Peltier coefficient, Pt, as:

$$\mathrm{Pt}(\mathrm{N}, \mathrm{r}_{\mathrm{d(a)}}, \mathrm{x}, \mathrm{T}) \equiv \mathrm{T} \times \mathrm{S}\ (\mathrm{V}). \tag{30}$$

One notes here that for given physical conditions N (or T) and for the decreasing $\xi_{\mathrm{n(p)}}$, since $\mathrm{VC1}(\mathrm{N}, \mathrm{r}_{\mathrm{d(a)}}, \mathrm{x}, \mathrm{T})$ and $\mathrm{Ts}(\mathrm{N}, \mathrm{r}_{\mathrm{d(a)}}, \mathrm{x}, \mathrm{T})$ are expressed in terms of $\frac{-\mathrm{dS}}{\mathrm{dN}^*}$ and $\frac{\mathrm{dS}}{\mathrm{dT}}$, one has: $[\mathrm{VC1}, \mathrm{Ts}] < 0$ for $\xi_{\mathrm{n(p)}} > \sqrt{\frac{\pi^2}{3}}$, $[\mathrm{VC1}, \mathrm{Ts}] = 0$ for $\xi_{\mathrm{n(p)}} = \sqrt{\frac{\pi^2}{3}}$, and $[\mathrm{VC1}, \mathrm{Ts}] > 0$ for $\xi_{\mathrm{n(p)}} < \sqrt{\frac{\pi^2}{3}}$, stating also that for $\xi_{\mathrm{n(p)}} = \sqrt{\frac{\pi^2}{3}}$:

(i) S, determined in Eq. (25), thus presents **a same minimum** $(\mathrm{S})_{\mathrm{min.}} = -\sqrt{\mathrm{L}} \simeq -1.563 \times 10^{-4} \left(\frac{\mathrm{V}}{\mathrm{K}}\right)$,

(ii) ZT, determined in Eq. (26), therefore presents **a same maximum:** $(\mathrm{ZT})_{\mathrm{max.}} = 1$, since the variations of ZT are expressed in terms of $[\mathrm{VC1}, \mathrm{Ts}] \times \mathrm{S}$, $\mathrm{S} < 0$.

Furthermore, it is interesting to remark that the (VC2)-coefficient is related to our generalized Einstein relation (24) by:

$$\frac{\mathrm{k_B}}{\mathrm{q}} \times \mathrm{VC2}(\mathrm{N}, \mathrm{r}_{\mathrm{d(a)}}, \mathrm{x}, \mathrm{T}) \equiv -\frac{\partial S}{\partial \xi_{\mathrm{n(p)}}} \times \frac{\mathrm{D}(\mathrm{N}, \mathrm{r}_{\mathrm{d(a)}}, \mathrm{x}, \mathrm{T})}{\mu(\mathrm{N}, \mathrm{r}_{\mathrm{d(a)}}, \mathrm{x}, \mathrm{T})} \left(\frac{\mathrm{V}^2}{\mathrm{K}}\right), \quad \frac{\mathrm{k_B}}{\mathrm{q}} = \sqrt{\frac{3 \times \mathrm{L}}{\pi^2}}, \tag{31}$$

according, in this work, with the use of our Eq. (25), to:

$$\mathrm{VC2}(\mathrm{N}, \mathrm{r}_{\mathrm{d(a)}}, \mathrm{x}, \mathrm{T}) \equiv -\frac{\mathrm{D}(\mathrm{N}, \mathrm{r}_{\mathrm{d(a)}}, \mathrm{x}, \mathrm{T})}{\mu(\mathrm{N}, \mathrm{r}_{\mathrm{d(a)}}, \mathrm{x}, \mathrm{T})} \times 2 \times \frac{(\mathrm{ZT})_{\mathrm{Mott}} \times [1-(\mathrm{ZT})_{\mathrm{Mott}}]}{[1+(\mathrm{ZT})_{\mathrm{Mott}}]^2} \ (\mathrm{V}).$$

Of course, our relation (31) is reduced to: $\frac{\mathrm{D}}{\mu}$, VC1 and VC2, being determined respectively by Equations (24, 27, 28). This may be a new result.

CONCLUDING REMARKS

Some important concluding remarks can be repoted as follows.

(1) As observed in Equations (3, 5, 6), the critical impurity density $\mathrm{N}_{\mathrm{CDn(CDp)}}$, defined by the generalized Mott criterium in the metal-insulator transition (**MIT**), is just the density of electrons (holes), localized in the exponential conduction (valence)-band tail (**EBT**), $\mathrm{N}^{\mathrm{EBT}}_{\mathrm{CDn(CDp)}}$, being obtained with a precision of the order of $\mathbf{3 \times 10^{-7}}$, respectively, as given in our recent works.[3] Therefore, the effective electron (hole)-density can be defined as: $\mathrm{N}^* \equiv \mathrm{N} - \mathrm{N}_{\mathrm{CDn(CDp)}} \simeq \mathrm{N} - \mathrm{N}^{\mathrm{EBT}}_{\mathrm{CDn(CDp)}}$, N being the total impurity density, as that observed in the compensated crystals.

(2) The ratio of the inverse effective screening length $\mathrm{k}_{\mathrm{sn(sp)}}$ to Fermi wave number $\mathrm{k}_{\mathrm{Fn(kp)}}$ at 0 K, $\mathrm{R}_{\mathrm{sn(sp)}}(\mathrm{N}^*)$, defined in Eq. (7), is valid at any N^*.

(3) The Fermi energy for any N and T, $\mathrm{E}_{\mathrm{Fn(Fp)}}$, determined in Eq. (11) with a precision of the order of 2.11×10^{-4} [9], affecting all the expressions of optical, and electrical-and-thermoelectric coefficients.

(4) One further notes that: (i) $\sigma_{\mathrm{O}}(\mathrm{N}, \mathrm{r}_{\mathrm{d(a)}}, \mathrm{x}, \mathrm{T}, \mathrm{E})$, given in Eq. (18), increases with increasing E for given $(\mathrm{N}, \mathrm{r}_{\mathrm{d(a)}}, \mathrm{x}, \mathrm{T}$)-physical conditions, (ii) as $\mathrm{E} = \mathrm{E}_{\mathrm{gn1(gp1)}}(\mathrm{N}, \mathrm{r}_{\mathrm{d(a)}}, \mathrm{x}, \mathrm{T})$, $\sigma_{\mathrm{O}}(\mathrm{N}, \mathrm{r}_{\mathrm{d(a)}}, \mathrm{x}, \mathrm{T}, \mathrm{E}) = 0$, as investigated in our previous work[2], and (iii) as $\mathrm{E} \to \infty$, the above result is reduced to the highest one, σ_{HO}, as given in Eq. (19).

(5) Further, from Eq. (16), by basing on: $\mathrm{n}(\mathrm{E}, \mathrm{r}_{\mathrm{d(a)}})$ and $\sigma_{\mathrm{O}}(\mathrm{N}, \mathrm{r}_{\mathrm{d(a)}}, \mathrm{x}, \mathrm{T}, \mathrm{E})$, determined in Equations (17, 18), one obtains: (i) as $\mathrm{E} = \mathrm{E}_{\mathrm{gn1(gp1)}}$, one gets: $\kappa(\mathrm{E}) = 0$, $\varepsilon_2(\mathrm{E}) = 0$, $\propto(\mathrm{E}) = 0$, and $\sigma_{\mathrm{O}}(\mathrm{E}) = 0$, as those obtained in our previous work[2], and (ii) as $\mathrm{E} \to \infty$, $\mathrm{n}(\mathrm{E}) \to$ constant, $\sigma_{\mathrm{O}}(\mathrm{E}) \to$ constant, $\propto(\mathrm{E}) \to$ constant, $\mathrm{R}(\mathrm{E}) \to$ constant, $\kappa(\mathrm{E}) \to 0$, $\varepsilon_1(\mathrm{E}) \to$ constant, and $\varepsilon_2(\mathrm{E}) \to 0$, as those obtained in our previous work.[2]

(6) Furthermore, for any given x, $r_{d(a)}$ and N (or T), with increasing T (or decreasing N), one obtains: (i) for $\xi_{n(p)} = \sqrt{\frac{\pi^2}{3}} \simeq 1.8138$, while the numerical results of the Seebeck coefficient S present a same minimum $(S)_{min.} \left(\simeq -1.563 \times 10^{-4} \frac{V}{K}\right)$, those of the figure of merit ZT show a same maxi**mum** $(ZT)_{max.} = 1$, (ii) for $\xi_{n(p)} = 1$, the numerical results of S, ZT, the Mott figure of merit $(ZT)_{Mott}$, the first Van-Cong coefficient VC1, and the Thomson coefficient Ts, present the same results: $-1.322 \times 10^{-4} \frac{V}{K}$, 0.715, 3.290, $1.105 \times 10^{-4} \frac{V}{K}$, and $1.657 \times 10^{-4} \frac{V}{K}$, respectively, and finally (iii) for $\xi_{n(p)} = \sqrt{\frac{\pi^2}{3}} \simeq 1.8138$, $(ZT)_{Mott} = 1$, as those given in our recent work.[1] It seems that these same results could represent **a new law in the thermoelectric properties, obtained in the degenerate case ($\xi_{n(p)} \geq 0$)**.

(7) Finally, our electrical-and-thermoelectric relation is given in Eq. (31) by: $\frac{k_B}{q} \times VC2(N, r_{d(a)}, x, T) \equiv -\frac{\partial S}{\partial \xi_{n(p)}} \times \frac{D(N, r_{d(a)}, x, T)}{\mu(N, r_{d(a)}, x, T)} \left(\frac{V^2}{K}\right)$, $\frac{k_B}{q} = \sqrt{\frac{3 \times L}{\pi^2}}$, according, in this work, to:
$VC2(N, r_{d(a)}, x, T) \equiv -\frac{D(N, r_{d(a)}, x, T)}{\mu(N, r_{d(a)}, x, T)} \times 2 \times \frac{(ZT)_{Mott} \times [1-(ZT)_{Mott}]}{[1+(ZT)_{Mott}]^2}$ (V), being reduced to: $\frac{D}{\mu}$, VC1 and VC2, determined respectively in Equations (24, 27, 28). This can be **a new result**.

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