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# OPTICAL PHENOMENON - ELECTRICAL PHENOMENON TRANSITION IN N(P)-TYPE DEGENERATE "COMPENSATED" A(1-X)B(X)-CRYSTALLINE ALLOY (1)

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## ABSTRACT

In the $\mathbf{n^+(p^+)} - A_{(1-x)}B_x$- crystalline alloy, $0 \le x \le 1$, 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 at $T \ge 0$ K, $E_{Fn(Fp)}(E_{Fno(Fpo)})$, determined in Eq. (11) and accurate with a precision of the order of $2.11 \times 10^{-4}$[9], affecting all the expressions of optical, and electrical-and-thermoelectric coefficients, are now investigated, by basing on our physical model, and Fermi-Dirac distribution function, as those given in our recent works.[1, 2] In the following, for given physical conditions, all the optical coefficients are expressed as functions of the effective photon energy : $E^* \equiv E - E_{gn1(gp1)}$, E and $E_{gn1(gp1)}$ being the photon energy and the optical band gap. Then, some important remarks can be repoted as follows.

-From our essential optical conductivity model, $\sigma_O(E^*)$, determined in Eq. (18), all the optical coefficients and electrical-and-thermoelectric ones are determined, as those given in Equations (19a-19d, 20a-20d).

-In particular, from the optical-and-electrical transformation duality given in Eq. (15), $E = E_{gn1(gp1)} + E_{Fn(Fp)}(E_{Fno(Fpo)})$ , according to the optical phenomenon-electrical

phenomenon transition effect, $\sigma_O$ has a same form with that of the electrical conductivity, $\sigma$, as given in Eq. (20a), and in our recent work[1], suggesting many important concluding remarks on the electrical-and-thermoelectric coefficients, as those given in Equations (20a, 21-30) and in our recent work.[1]

**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 $2.11 \times 10^{-4}$ [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, 20a),

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 $\mathbf{3 \times 10^{-7}}$ , 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) From our basical optical conductivity model given in Eq. (18), all the optical and optical, and electrical-and-thermoelectric coefficients are well determined. In particular, from the optical-and-electrical transformation duality given in Eq. (15), according to the optical phenomenon- electrical phenomenon transition effect, the optical conductivity, $\sigma_O$ , determined in Eq. (18), has the same form with that of the electrical conductivity, σ, as given in Eq. (20a), and in our recent work.[1]

(4) From Equations (20a, 21-30), 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 ($\xi_{n(p)} \geq 0$).**

**(5)** Finally, our electrical-and-thermoelectric relation is given in Eq. (31) by:

$\frac{k_B}{q} \times VC2\left(N, r_{d(a)}, x, T\right) \equiv -\frac{\partial S}{\partial \xi_{n(p)}} \times \frac{D(N,r_{d(a)},x,T)}{\mu(N,r_{d(a)},x,T)} \left(\frac{V^2}{K}\right)$, $\frac{k_B}{q} = \sqrt{\frac{3\times L}{\pi^2}}$ , according, in this work, to:

$VC2\left(N, r_{d(a)}, x, T\right) \equiv -\frac{D(N,r_{d(a)},x,T)}{\mu(N,r_{d(a)},x,T)} \times 2 \times \frac{(ZT)_{Mott}\times[1-(ZT)_{Mott}]}{[1+(ZT)_{Mott}]^2}$ (V) , being reduced to: $\frac{D}{\mu}$ , VC1 and VC2, determined respectively in Equations (24, 27, 28). This should be **a new result**.

In the following, many important sections are presented in order to investigate all the optical coefficients and electrical-and-thermoelectric ones, given in the $\mathbf{n^+(p^+)} - A_{(1-x)}B_x$ -crystalline alloy at any temperature $T(\geq 0\ K)$.

## 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: $\mathbf{r_{do(ao)}}$=$\mathbf{r_A}$, the effective averaged numbers of equivalent conduction (valence)-bands by : $g_{c(v)}$ , the unperturbed reduced 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) $\alpha$, $\alpha_o = 0$. Further, the two important equations, used to determine the $\alpha$ -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 $E_{gn(gp)}\left(r_{d(a)}, x\right)$, and the effective donor (acceptor)-ionization energy $E_{d(a)}\left(r_{d(a)}, x\right)$ in absolute values, obtained in the effective Bohr model, which is represented respectively by : $\pm\left[\Delta\alpha(r_{d(a)}, x)\right]_{n(p)}$,

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

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

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

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 $\boldsymbol{\varepsilon(r_{d(a)},x)}$-law**,

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

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 $\boldsymbol{\varepsilon(r_{d(a)},x)}$-law**,

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

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 $\boldsymbol{\varepsilon(r_{d(a)},x)}$-law.**

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

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

**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]:

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

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 :

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

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

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

**Explaining thus the existence of the Mott's criterium**.

Furthermore, by using $M_{n(p)} = 0.25$, according to the empirical Heisenberg parameter $\boldsymbol{\mathcal{H}_{n(p)}} = \mathbf{0.47137}$, 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** , $\mathbf{N^{EBT}_{CDn(CDp)}}$ , 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 $E_{gno(gpo)}\left(r_{d(a)}, x\right)$ , $N_{CDn(NDp)}(r_{d(a)}, x)$ and $N^{EBT}_{CDn(CDp)}(r_{d(a)}, x)$ increase, affecting strongly all the optical properties and the electrical-and-thermoelectric ones, 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:

$\gamma \times r_{sn(sp)}(N^{*}) \equiv \frac{k_{Fn(Fp)}^{-1}}{a_{Bn(Bp)}} < 1$ , $r_{sn(sp)}(N, r_{d(a)}, x) \equiv \left(\frac{3g_{c(v)}}{4\pi N^{*}}\right)^{1/3} \times \frac{1}{a_{Bn(Bp)}(r_{d(a)},x)}$ , being proportional to $N^{*-1/3}$. Here, $\gamma = (4/9\pi)^{1/3}$, $k_{Fn(Fp)}(N^{*}) \equiv \left(\frac{3\pi^{2} N^{*}}{g_{c(v)}}\right)^{\frac{1}{3}}$ is the Fermi wave, $g_{c(v)}$ being the effective averaged numbers of equivalent conduction (valence)-bands, and $a_{Bn(Bp)}(r_{d(a)},x)$ is determined in Eq. (2), in which $m_{c(v)}(x)$ is replaced by the relative effective carrier mass, defined by: $m_{r}(x) \equiv \frac{m_{c}(x) \times m_{v}(x)}{m_{c}(x)+m_{v}(x)}$.

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

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

**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

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

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

Secondly, 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

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

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:

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

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

BAND GAP NARROWING (BGN) BY N AND BY T

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

$$\Delta E_{gn(gp);N}(N^*, r_{d(a)}, x) \simeq a_1 + \frac{\varepsilon_0(x)}{\varepsilon(r_{d(a)}, x)} \times N_r^{\frac{1}{3}} + a_2 \times \frac{\varepsilon_0(x)}{\varepsilon(r_{d(a)}, x)} \times N_r^{\frac{1}{3}} \times \left(2.503 \times [-E_{CE}(r_{sn(sp)})] \times r_{sn(sp)}\right) + a_3 \times \left[\frac{\varepsilon_0(x)}{\varepsilon(r_{d(a)}, x)}\right]^{\frac{5}{4}} \times \sqrt{\frac{m_p}{m_r}} \times N_r^{\frac{1}{4}} + 2a_4 \times \left[\frac{\varepsilon_0(x)}{\varepsilon(r_{d(a)}, x)}\right]^{\frac{1}{2}} \times N_r^{\frac{1}{2}} + 2a_5 \times \left[\frac{\varepsilon_0(x)}{\varepsilon(r_{d(a)}, x)}\right]^{\frac{3}{2}} \times N_r^{\frac{1}{6}},\ N_r = \frac{N^*}{9.999 \times 10^{17}\,cm^{-3}}, \tag{10a}$$

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

Therefore, 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]:

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

## 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 $2.11 \times 10^{-4}$, is found to be given by:

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

where u is the reduced electron density, $u(N, r_{d(a)}, x, T) \equiv \frac{N^*}{N_{c(v)}(T,x)}$ , $N_{c(v)}(T,x) = 2g_{c(v)} \times \left(\frac{m_r(x) \times m_o \times k_B T}{2\pi\hbar^2}\right)^{\frac{3}{2}}$ $(cm^{-3})$ , $F(u) = au^{\frac{2}{3}}\left(1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}}\right)^{-\frac{2}{3}}$, $a = \left[3\sqrt{\pi}/4\right]^{2/3}$, $b = \frac{1}{8}\left(\frac{\pi}{a}\right)^2$ , $c = \frac{62.3739855}{1920}\left(\frac{\pi}{a}\right)^4$ , 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 $\mathbf{u \longrightarrow 0}$**, the limiting non-degenerate condition**, and in the very degenerate case ($u \gg 1$), one gets: $E_{Fn(Fp)}(u \gg 1) = k_B T \times F(u) = k_B T \times au^{\frac{2}{3}}\left(1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}}\right)^{-\frac{2}{3}} \simeq \frac{\hbar^2 \times k_{Fn(Fp)}^2(N^*)}{2 \times m_r(x) \times m_o}$ as $\mathbf{u \longrightarrow \infty}$**, 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: $E_{Fno(Fpo)}(N^*) \equiv \frac{\hbar^2 \times k_{Fn(Fp)}^2(N^*)}{2 \times m_r(x) \times m_o}$, 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 $\xi_{n(p)}\left(N, r_{d(a)}, x, T\right)$ [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:

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

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

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

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

, where $C_p^{\beta} \equiv p(p-1) \dots (p-\beta+1)/\beta!$ and the integral $I_{\beta}$ 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 $\beta$. 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:

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

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 the following Table 1, being needed to determine all the following optical and 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.

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

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), One has:

(i) in the electrical phenomenon (EP), the reduced band gap is defined by:

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

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 Equations (10a, 10b), and

(ii) in the optical phenomenon (OP), the photon energy is defined by: $E \equiv \hbar\omega$, and the optical band gap, by: $E_{gn1(gp1)} \equiv E_{gn2(gp2)} + E_{Fn(Fp)}$. Therefore, for $E \geq E_{gn1(gp1)}$, the effective photon energy $E^*$ is found to be given by:

$$E^* \equiv E - E_{gn1(gp1)} = E - \left(E_{gn2(gp2)} + E_{Fn(Fp)}\right) \geq 0. \quad (14)$$

From above Equations, an optical-and-electrical transformation duality means that:

$E^* \equiv E - E_{gn1(gp1)}$, given in the OP, is reduced, as $E = E_{gn1(gp1)} + E_{Fn(Fp)}\left[E_{Fno(Fpo)}\right]$, given in the EP, in which $m_r(x)$ is now replaced by $m_{c(v)}(x)$, to: $E^* \equiv E - E_{gn1(gp1)} = E_{Fn(Fp)}\left[E_{Fno(Fpo)}\right]$, and reciprocally, replacing $m_{c(v)}(x)$ by $m_r(x)$ given in the OP. (15)

Eq. (15) thus shows that, in 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.

Optical Coefficients

The optical properties for any medium can be described by the complex refraction: $\mathbb{N} \equiv n - i\kappa$, n and $\kappa$ 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 $\propto$, and the joint density of states by:

$$JDOS_{n(p)}(E) \equiv \frac{1}{2\pi^2} \times \left(\frac{2m_r}{\hbar^2}\right)^{3/2} \times \left[\frac{E - E_{gn1(gp1)}(T)}{E - E_{gn1(gp1)}(T=0)}\right]^2 \times \sqrt{E_{Fno(Fpo)}},$$ and

$F(E) \equiv \frac{\hbar q^2 \times |v(E)|^2}{n(E) \times cE \times \varepsilon_{free\ space}}$, one gets[2]:

$$\propto(E) = JDOS_{n(p)}(E) \times F(E) = \frac{E \times \varepsilon_2(E)}{\hbar c n(E)} = \frac{2E \times \kappa(E)}{\hbar c} = \frac{4\pi\sigma_O(E)}{cn(E) \times \varepsilon_{free\ space}}, \varepsilon_1 \equiv n^2 - \kappa^2, \varepsilon_2 \equiv 2\kappa n,$$

and $R(E) \equiv \frac{[n-1]^2 + \kappa^2}{[n+1]^2 + \kappa^2}$. (16)

It should be noted that, such the above joint density of states yeilds: (i) as $E = E_{gn1(gp1)}(T)$, $JDOS_{n(p)}(E) = 0$, and (ii) as $E \to \infty$, $JDOS_{n(p)}(E) \to \frac{1}{2\pi^2} \times \left(\frac{2m_r}{\hbar^2}\right)^{3/2} \times \sqrt{E_{Fno(Fpo)}}$. Further,

$\varepsilon_{\text{free space}}$ is the permittivity of the free space, -q is the charge of the electron, $|v(E)|$ is the matrix elements of the velocity operator between valence (conduction)-and-conduction (valence) bands, and the refraction index n is found to be defined by[2]:

$$n(E,\ r_{d(a)}) \equiv n_\infty(r_{d(a)}) + \sum_{i=1}^{4} \frac{B_{oi}E + C_{oi}}{E^2 - B_1 E + C_i} \to n_\infty\left(r_{d(a)}\right), \text{ as } E \to \infty. \tag{17}$$

Here, the optical conductivity $\sigma_O$ can be defined and expressed in terms of the kinetic energy of the electron (hole), $E_k \equiv \frac{\hbar^2 \times k^2}{2\times m_r(x)\times m_o}$, 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, from above equations (16, 17), our optical conductivity model can be assumed to be as:

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

which gives: $\sigma_O\left(E = E_{gn1(gp1)}(T)\right) = 0$, and $\sigma_O(E \to \infty) = \text{Constant}$ for given $\left(N, r_{d(a)}, x, T\right)$ – physical conditions, as those given in Ref. [2].

Here, $\frac{q^2}{\pi\times\hbar} = 7.7480735 \times 10^{-5}\ \text{ohm}^{-1}$, $A_{n(p)}(N^*) = \frac{E_{Fno(Fpo)}(N^*)}{\eta_{n(p)}(N^*)}$, $R_{sn(sp)}(N^*) \equiv \frac{k_{sn(sp)}}{k_{Fn(Fp)}}$.

This result (18) should be new, in comparison with that, obtained from an improved Forouhi-Bloomer parameterization, as given in our previous work.[2]

Using Equations (16-18), one obtains:

$$\frac{|v(E)|^2}{E} = \frac{8\pi^2\hbar}{(2m_r)^{3/2}\times\sqrt{E_{Fno(Fpo)}}} \times \left[\frac{k_{Fn(Fp)}(N^*)}{R_{sn(sp)}(N^*)} \times \left[k_{Fn(Fp)}(N^*) \times a_{Bn(Bp)}\left(r_{d(a)}, x\right)\right] \times \sqrt{A_{n(p)}(N^*)}\right] \times G_2\left(N, r_{d(a)}, x, T\right), \tag{19a}$$

$$\kappa(E) = \frac{2q^2}{n(E)\times\varepsilon_{\text{free space}}\times E} \times \left[\frac{k_{Fn(Fp)}(N^*)}{R_{sn(sp)}(N^*)} \times \left[k_{Fn(Fp)}(N^*) \times a_{Bn(Bp)}\left(r_{d(a)}, x\right)\right] \times \sqrt{A_{n(p)}(N^*)}\right] \times G_2\left(N, r_{d(a)}, x, T\right) \times \left[\frac{E - E_{gn1(gp1)}(T)}{E - E_{gn1(gp1)}(T=0)}\right]^2, \tag{19b}$$

which gives: $\kappa\left(E = E_{gn1(gp1)}(T)\right) = 0$, and $\kappa(E \to \infty) \to 0$, as those given in Ref. [2],

$$\varepsilon_2(E) = \frac{4q^2}{\varepsilon_{\text{free space}} \times E} \times \left[\frac{k_{Fn(Fp)}(N^*)}{R_{sn(sp)}(N^*)} \times \left[k_{Fn(Fp)}(N^*) \times a_{Bn(Bp)}\left(r_{d(a)}, x\right)\right] \times \sqrt{A_{n(p)}(N^*)}\right] \times G_2\left(N, r_{d(a)}, x, T\right) \times \left[\frac{E - E_{gn1(gp1)}(T)}{E - E_{gn1(gp1)}(T=0)}\right]^2, \quad (19c)$$

which gives: $\varepsilon_2\left(E = E_{gn1(gp1)}(T)\right) = 0$, and $\varepsilon_2(E \to \infty) \to 0$, as those given in Ref. [2], and

$$\propto (E) = \frac{4q^2}{\hbar c n(E) \times \varepsilon_{\text{free space}}} \times \left[\frac{k_{Fn(Fp)}(N^*)}{R_{sn(sp)}(N^*)} \times \left[k_{Fn(Fp)}(N^*) \times a_{Bn(Bp)}\left(r_{d(a)}, x\right)\right] \times \sqrt{A_{n(p)}(N^*)}\right] \times G_2\left(N, r_{d(a)}, x, T\right) \times \left[\frac{E - E_{gn1(gp1)}(T)}{E - E_{gn1(gp1)}(T=0)}\right]^2 \ (\text{cm}^{-1}), \quad (19d)$$

which gives: $\propto \left(E = E_{gn1(gp1)}(T)\right) = 0$, and $\propto (E \to \infty) = \text{Constant}$, as those given in Ref.[2]

Using the optical-and-electrical transformation duality, given in Eq. (15), at $E = E_{gn1(gp1)} + E_{Fn(Fp)}\left[E_{Fno(Fpo)}\right]$, the optical conductivity, $\sigma_O$ given in Eq. (18), in which $m_r(x)$ is now replaced by $m_{c(v)}(x)$, has the same form with that of the electrical conductivity, σ, given in our recent work [1], for such an optical phenomenon-and- electrical phenomenon transition. So, from Equations (18, 19b, 19c, 19d), ones obtains respectively, as:

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

having the same form with that of $\sigma\left(N, r_{d(a)}, x, T\right)$,

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

$$\kappa(E) = \frac{2q^2}{n(E) \times \varepsilon_{\text{free space}} \times E} \times \left[\frac{k_{Fn(Fp)}(N^*)}{R_{sn(sp)}(N^*)} \times \left[k_{Fn(Fp)}(N^*) \times a_{Bn(Bp)}\left(r_{d(a)}, x\right)\right] \times \sqrt{A_{n(p)}(N^*)}\right] \times G_2\left(N, r_{d(a)}, x, T\right) \times \left(\frac{E_{Fn(Fp)}(N, r_{d(a)}, x, T)}{E_{Fno(Fpo)}(N, r_{d(a)}, x, T=0)}\right)^2, \quad (20b)$$

$$\varepsilon_2(E) = \frac{4q^2}{\varepsilon_{\text{free space}} \times E} \times \left[\frac{k_{Fn(Fp)}(N^*)}{R_{sn(sp)}(N^*)} \times \left[k_{Fn(Fp)}(N^*) \times a_{Bn(Bp)}\left(r_{d(a)}, x\right)\right] \times \sqrt{A_{n(p)}(N^*)}\right] \times G_2\left(N, r_{d(a)}, x, T\right) \times \left(\frac{E_{Fn(Fp)}(N, r_{d(a)}, x, T)}{E_{Fno(Fpo)}(N, r_{d(a)}, x, T=0)}\right)^2, \quad \text{and} \quad (20c)$$

$$\propto(E) = \frac{4q^2}{\hbar c n(E)\times\varepsilon_{\text{free space}}} \times \left[\frac{k_{Fn(Fp)}(N^*)}{R_{sn(sp)}(N^*)} \times \left[k_{Fn(Fp)}(N^*) \times a_{Bn(Bp)}(r_{d(a)},x)\right] \times \sqrt{A_{n(p)}(N^*)}\right] \times G_2(N,r_{d(a)},x,T) \times \left(\frac{E_{Fn(Fp)}(N,r_{d(a)},x,T)}{E_{Fno(Fpo)}(N,r_{d(a)},x,T=0)}\right)^2 \ (cm^{-1}). \quad (20d)$$

One notes that the electrical conductivity $\sigma(N,r_{d(a)},x,T)$, given in Eq. (2a), is a basical result, being used to determine other following electrical-and-thermoelectric coefficients.

## ELECTRICAL-AND-THERMOELECTRIC PROPERTIES

Here, if denoting, for majority electrons (holes), the thermal conductivity by $\sigma_T(N,r_{d(a)},x,T)$ in $\frac{W}{cm\times K}$, and the Lorenz number L by: $L = \frac{\pi^2}{3}\times\left(\frac{k_B}{q}\right)^2 = 2.4429637\ \left(\frac{W\times ohm}{K^2}\right) = 2.4429637\times10^{-8}\ (V^2\times K^{-2})$, then the well-known Wiedemann-Frank law states that the ratio, $\frac{\sigma_T}{\sigma}$, is proportional to the temperature T(K), as:

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

Further, the resistivity is found to be given by: $\rho(N,r_{d(a)},x,T)\equiv 1/\sigma(N,r_{d(a)},x,T)$, noting again that $N^*\equiv N-N_{CDn(NDp)}(r_{d(a)},x)$.

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 $\tau$ is related to $\sigma$ by[1]:

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

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

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

$r_H(N,r_{d(a)},x,T)\equiv\frac{\langle\tau^2\rangle_{FDDF}}{[\langle\tau\rangle_{FDDF}]^2} = \frac{G_4(y)}{[G_2(y)]^2}$, $y\equiv\frac{\pi}{\xi_{n(p)}(N,r_{d(a)},x,T)} = \frac{\pi k_B T}{E_{Fn(Fp)}(N,r_{d(a)},x,T)}$, and therefore, the Hall mobility yields:

$$\mu_H(N, r_{d(a)}, x, T) \equiv \mu(N, r_{d(a)}, x, T) \times r_H(N^*, T)\ (\frac{cm^2}{V\times s}), \tag{23}$$

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]:

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

where $D(N, r_{d(a)}, x, T)$ is the diffusion coefficient, $\xi_{n(p)}(u)$ is defined in Eq. (11), and the mobility $\mu(N, r_{d(a)}, x, T)$ 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:

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

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

**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:

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

Then, using Eq. (11), for the degenerate case, $\xi_{n(p)} \geq 0$, one gets, by putting

$$F_S(N, r_{d(a)}, x, T) \equiv \left[1 - \frac{y^2}{3\times G_2\left(y=\frac{\pi}{\xi_{n(p)}}\right)}\right],$$

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

$$-2\sqrt{L} \times \frac{\sqrt{(ZT)_{Mott}}}{1+(ZT)_{Mott}}\left(\frac{V}{K}\right) < 0, \quad (ZT)_{Mott} = \frac{\pi^2}{3\times\xi_{n(p)}^2}, \tag{25}$$

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:

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

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

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

$VC1(N, r_{d(a)}, x, T) \equiv -N^* \times \frac{dS}{dN^*}\left(\frac{V}{K}\right) = N^* \times \frac{\partial S}{\partial \xi_{n(p)}} \times -\frac{\partial \xi_{n(p)}}{\partial N^*}$, being equal to 0 for

$$\xi_{n(p)} = \sqrt{\frac{\pi^2}{3}}, \tag{27}$$

and the second Van-Cong coefficient, VC2, as:

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

the Thomson coefficient, Ts, by:

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

and the Peltier coefficient, Pt, as:

$$Pt(N, r_{d(a)}, x, T) \equiv T \times S\,(V). \quad (30)$$

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

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

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

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

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

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

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

Of course, our relation (31) is reduced to: $\frac{D}{\mu}$, 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.

In the $\mathbf{n^+(p^+)} - A_{(1-x)}B_x$- crystalline alloy, $0 \le x \le 1$, 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 $2.11 \times 10^{-4}$ [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, 20a),

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 $\mathbf{3 \times 10^{-7}}$ , 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) From our basical optical conductivity model given in Eq. (18), all the optical and optical, and electrical-and-thermoelectric coefficients are well determined. In particular, from the optical-and-electrical transformation duality given in Eq. (15), according to the optical phenomenon- electrical phenomenon transition effect, the optical conductivity, $\sigma_O$ , determined in Eq. (18), has the same form with that of the electrical conductivity $\sigma$, as given in Eq. (20a), and in our recent work.[1]

(4) From Equations (20a, 21-30), 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 ($\xi_{n(p)} \geq 0$).**

**(5)** 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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