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A Theoretical Estimate of the Temperature Dependence of Electron Concentration and Lorenz Number in the Spherically Symmetric Zone of Semiconductors

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An accurate approach is proposed for the temperature dependence of electron concentration and Lorenz number in the spherically symmetric zone of semiconductors. The evaluation includes more accurate analytical calculations over the study for two parameters of Fermi functions. Recently, a new analytical approach for the calculation of the two parameters of Fermi functions has been reported in terms of summations of binomial coefficients and incomplete gamma functions. The method is applied to the case of the Ge and GaAs semiconductors, which can determine the electron concentration and Lorenz number as a function of temperature variation. The results obtained by the suggested and numerical methods are satisfactory for a wide range of temperatures. The method descriptions are very well for the investigation of other thermoelectric effects over the whole temperature ranges.

Keywords: semiconductor, electron concentration, two parameter Fermi functions, thermoelectric.

1. INTRODUCTION

The thermoelectric and thermomagnetic effects are important both as a means of determining the characterization of semiconductors materials and practical applications like all type of engineering science and technology [1 – 7]. Note that all thermoelectric phenomena (Thomson, Seebeck, Peltier effects etc.) in semiconductors are effective much more strongly than in metals. There is a wide class of semiconductors in which the conduction band is spherically symmetric but nonparabolic. The spherically symmetric zone is characterized by the fact that the energy in such a zone depends only on the modulus of the wave vector $\left|\vec{k}\right| = k$ [3 – 6].

The electron concentration and other thermoelectric effects of semiconductors were studied in many papers [8 – 23]. In [9], an effective approach has been proposed for predicting the temperature dependence of Hall electron concentration and mobility in n-GaN. The authors in work [10] have reported *n(T)* in type converted Si by using the method presented in the article [11]. Kumar et al. [24] have done a detailed analysis of the experimental determination methods of the Lorenz number in metals, semi-metals, alloys and degenerate semiconductors. In studies [25, 26] authors proposed as an alternative the first-principles approach to the evaluation of Lorenz numbers for complex thermoelectric materials. As seen from reported researches the majority of these have included semi-empirical or experimental methods. By applying Fermi-Dirac statistics, the general analytical formulas have been presented for the thermoelectric effects and electron concentration which these formulas are expressed by two parameters of Fermi functions [6 – 8]. Because it is difficult to generate an analytical formula for the two parameters Fermi function, the application of these formulas to date is very limited. In the literature, there are few theoretical studies, which have been applied for the evaluation of the two parameters of Fermi functions [6]. Very recently in the study [27 – 29], a full analytical formula for the two parameters of Fermi functions was developed and implemented.

In the present work, the electron concentration and Lorenz number are evaluated for the spherically symmetric zone of semiconductors by using the two parameters of Fermi functions formulae. The analytical formula is presented for Lorenz number and electron concentration which are used to obtain knowledge of the electrical conductance performance of semiconductor materials in arbitrary temperature ranges. Finally, the approach is used for calculations of electron concentration and Lorenz number for the spherically symmetric zone of the semiconductors materials Ge and GaAs.

2. EXPERIMENTAL SECTION

2.1. Definition and general analytical expressions

The electron concentration and Lorenz Number for the spherically symmetric zone of the semiconductors are expressed using the following formulae, respectively [6-8]:

$$n = \frac{(2m_n k_B T)^{3/2}}{3\pi^2\hbar^3} I^0_{3/2,0}(\eta,\beta); \tag{1}$$

and

$$L(r,\eta,\beta) = A(r,\eta,\beta)\left(\frac{k_B}{e}\right)^2, \tag{2}$$

where

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$$A(r,\eta,\beta)=\frac{I^2_{r+1,2}(\eta,\beta)}{I^0_{r+1,2}(\eta,\beta)}+\left(\frac{I^1_{r+1,2}(\eta,\beta)}{I^0_{r+1,2}(\eta,\beta)}\right)^2, \tag{3}$$

where m_n is the effective mass of the electron, $\hbar$ is the Planck constant, k_B is the Boltzmann coefficient, e is the charge electron, T is the absolute temperature, η is the reduced chemical potential, the parameter $\beta=\frac{k_BT}{\varepsilon_g}$ characterizes the non-standard zone and ε_g is the energy gap and the quantity $I^m_{n,k}(\eta,\beta)$ is two-parameter Fermi functions and defined as [6]:

$$I^m_{nk}(\eta,\beta)=\int_0^\infty\frac{x^m(x+\beta x^2)^n e^{x-\eta}}{(1+e^{x-\eta})^2(1+2\beta x)^k}dx\,. \tag{4}$$

As seen from studies [5 – 8] all thermoelectric effects evaluation has been reduced to two parameters of Fermi functions. Therefore, the analytical relation for two parameters of Fermi functions is important for accurate determining the thermoelectric effects of semiconductors. Earlier the authors developed a new analytical model for the accurate calculation of two parameters of Fermi functions [27] as follows: for $n\neq 0,\ k\neq 0, m\neq 0$

$$I^m_{nk}(\eta,\beta)=e^{-\eta}\lim_{N\to\infty}\sum_{i=0}^{N}f_i(-k)\times\begin{cases}\sum\limits_{j=0}^{n}f_j(n)\left[\beta^{i+j}2^iP_{m+n+i+j}\left(\eta,\frac{1}{2\beta}\right)\right.\\ \left.+\frac{\beta^{j-k-i}}{2^{k+i}}Q_{m+n-k-i+j}\left(\eta,\frac{1}{2\beta}\right)\right] & for\ n\,\text{integer}\\ \lim\limits_{N\to\infty}\sum\limits_{j=0}^{N}f_j(n)\left[\beta^{i+j}2^iP_{m+n+i+j}\left(\eta,\frac{1}{2\beta}\right)+\right.\\ \left.\frac{\beta^{n-j-k-i}}{2^{k+i}}Q_{m+2n-k-i+j}\left(\eta,\frac{1}{2\beta}\right)\right] & for\ n\,\text{noninteger}\end{cases}; \tag{5}$$

for $n=0,\ k=0\ and\ m\neq 0$

$$I^m_{00}(\eta,\beta)=e^{-\eta}\times\begin{cases}\lim\limits_{N\to\infty}\sum\limits_{i=0}^{N}\frac{f_i(-2)e^{i\eta}}{(1+i)^{m+1}}[(-1)^{m+1}\gamma(m+1,-(1+i)\eta)\\ \quad+e^{2\eta}\Gamma(m+1,(1+i)\eta)] & for\ \eta>0\\ \lim\limits_{N\to\infty}\sum\limits_{i=0}^{N}f_i(-2)\frac{e^{\eta(2+i)}\Gamma(m+1)}{(1+i)^{m+1}} & for\ \eta<0\end{cases}; \tag{6}$$

for $n\neq 0,\ k=0,\ m=0\ and\ \eta>0$

$$\mathrm{I}^0_{n0}(\eta,\beta)=e^{-\eta}\times\begin{cases}\sum\limits_{i=0}^{n}f_i(n)\beta^iL_{n+i}(\eta) & for\ n\ \text{integer}\\ \lim\limits_{N\to\infty}\sum\limits_{i=0}^{N}f_i(n)[\beta^iP_{n+i}(\eta,1/\beta)+\beta^{n-i}\\ \times Q_{2n-i}(\eta,1/\beta)] & for\ n\ \text{noninteger}\end{cases}; \tag{7}$$

for $n\neq 0,\ k=0,\ m=0\ and\ \eta<0$

$$\mathrm{I}^0_{n0}(\eta,\beta)=e^{-\eta}\times\begin{cases}\sum\limits_{i=0}^{n}f_i(n)\beta^i\lim\limits_{N\to\infty}\sum\limits_{j=0}^{N}f_j(-2)\\ \times\frac{e^{(2+j)\eta}\Gamma(n+i+1)}{(1+j)^{n+i+1}} & for\,n\,\text{integer}\\ \lim\limits_{N\to\infty}\sum\limits_{i=0}^{N}f_i(n)\sum\limits_{j=0}^{N}f_j(-2)e^{(2+j)\eta}\\ \left[\frac{\beta^i\gamma(n+i+1,(1+j)/\beta)}{(1+j)^{n+i+1}}\right.\\ \left.+\frac{\Gamma(2n-i+1,(1+j)/\beta)}{\beta^{i-n}(1+j)^{2n-i+1}}\right] & for\,n\,\text{noninteger}\end{cases}, \tag{8}$$

where N is upper limit of summations and is binomial coefficient defined as:

$$F_m(n)=\frac{1}{m!}\prod_{i=0}^{m-1}(n-i)\,. \tag{9}$$

The quantities $\Gamma(\alpha)$, $\Gamma(\alpha,x)$ and $\gamma(\alpha,x)$ are the incomplete Gamma functions defined by [30]:

$$\Gamma(\alpha)=\int_0^\infty t^{\alpha-1}e^{-t}dt\,; \tag{10}$$

$$\Gamma(\alpha,x)=\int_x^\infty t^{\alpha-1}e^{-t}dt\,; \tag{11}$$

and

$$\gamma(\alpha,x)=\int_0^x t^{\alpha-1}e^{-t}dt\,. \tag{12}$$

See Ref. [27] for the exact definition of the auxiliary functions $P_n(p, q)$, $Q_n(p, q)$ and $L_n(p)$ occurring in the Eq. 5 and Eq. 7. Also, for evaluation of incomplete Gamma functions, is described in [31, 32].

3. NUMERICAL RESULTS AND DISCUSSION

As seen from the studies in the literature, the proposed theoretical approaches to evaluating the temperature dependence of the electron concentration and Lorenz number of materials yield appropriate results in the restricted ranges of temperature. A new alternative evaluation method of the electron concentration and Lorenz Number for the spherically symmetric zone of the semiconductors is developed based on two parameters Fermi functions. The method applied in this research is based on kinetic theory, which simplifies the calculation of thermoelectric effects. In this study, the two parameters of Fermi functions are calculated with Eq. 4 – Eq. 8 developed in Ref. [27]. To demonstrate the usefulness of this approach, a computer program using Mathematica 10.0 compiler is established for the calculation of the electron concentration and Lorenz number. The comparison results of the temperature dependences of the electron concentration and Lorenz Number of the Ge and GaAs obtained from the proposed and Mathematica 10.0 numerical methods are shown in Fig. 1 – Fig. 4.

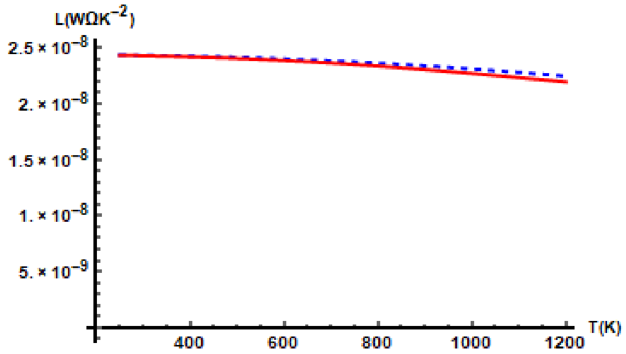

Fig. 1. The temperature dependence of Lorenz number of Ge (solid red line – mathematical numerical results, blue dashed line- results of this study)

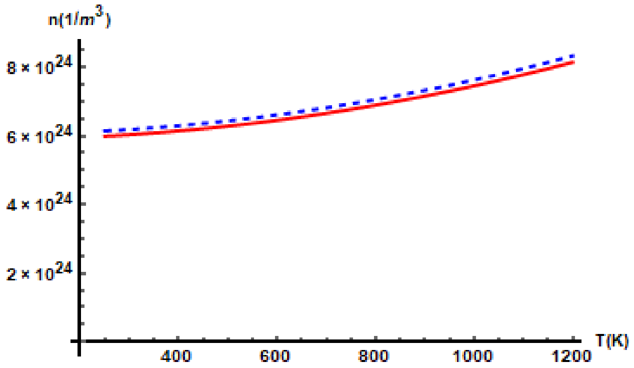

Fig. 2. The temperature dependence of electron concentration of Ge (solid red line – mathematical numerical results, blue dashed line- results of this study) of Ti-6Al-4V and MWCNT composite corrosion specimen

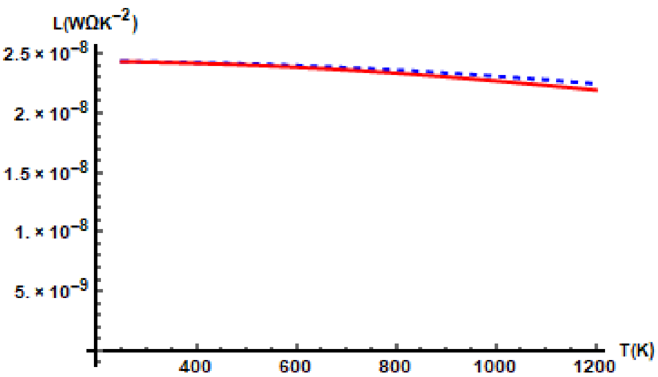

Fig. 3. The temperature dependence of Lorenz number of GaAs (solid red line – mathematical numerical results, blue dashed line- results of this study)

As seen from the figures, in the wide range temperature the calculated results are satisfactory. Also, it is shown from figures that the Lorenz number decrease with increasing temperature for Ge and GaAs semiconductors but the electron concentration vice versa. To our knowledge, there are no results in the literature on the wide range of temperature behavior of the electron concentration and Lorenz number.

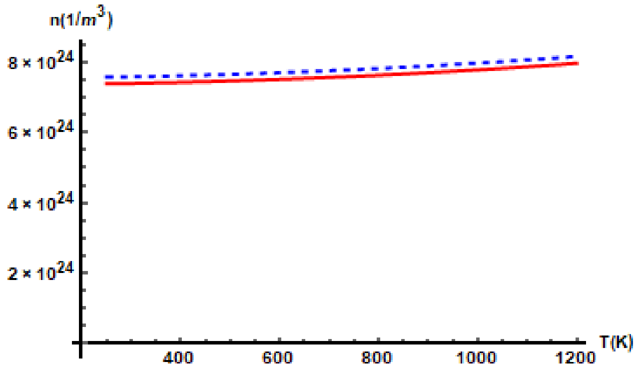

Fig. 4. The temperature dependence of electron concentration of GaAs (solid red line – mathematical numerical results, blue dashed line- results of this study)

This study provides an advancement in accurately calculating the temperature dependence of the electron concentration and Lorenz number for an arbitrary range of temperatures. Using data of the Lorent numbers for all the temperature values, allows us to follow the change of thermal and electrical conductivity of electronic materials according to temperature. It is well known that the determination of the thermal effects of thermopower materials with the variation of temperature is important in its uses in technological devices. All calculations have been developed for Ge and GaAs semiconductors with the parameters: $\varepsilon_{gGe} = 0.66\,eV$, $\varepsilon_{FGe} = 0.33\,eV$ and $\varepsilon_{gGaAs} = 1.424\,eV$, $\varepsilon_{FGaAs} = 0.712\,eV$, $k = 1.3806504E-23\,JK^{-1}$ and $e = 1.6021766x10^{-19}\,C$, $r = 1$. All present calculations were carried in SI unit systems. We note that in the study [29], the temperature dependence of the Lorenz number has been studied in the case of the scattering of acoustic phonons *r = 0*. In the present work, the evaluations of the electron concentration and Lorenz number have been done in the case of scattering on optical phonons *r = 1*. Consideration of the suggested method is not restricted by evaluation of the electron concentration and Lorenz number and provides a comprehensive study of other thermoelectric and thermomagnetic effect in semiconductors and materials.

4. CONCLUSIONS

In conclusion, we proposed a general analytical approach to calculate the electron concentration and Lorenz number for the spherically symmetric zone of the semiconductors. This work enables new developments in the evaluation of thermoelectric effects of metals, semi-metals, alloys and semiconductor materials in a wide range of temperatures. The present work is effective in evaluating the thermoelectric properties of materials from low temperature to high temperature which is the novelty of this study.

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