Thermoelectric Behavior of Silicon Nano Wire for Acoustic Phonon Scattering Including Multi Sub-Band Effect

Mahendra Pratap Singh[1]

[1]*Professor, Rajkiya Mahila Mahavidyalaya Shahganj Jaunpur Uttar Pradesh India*

Corresponding Author: singhmps74@gmail.com

***Abstract*: Thermoelectric power generation is non-conventional source of energy. Thermoelectric power can be increased by optimisation of figure of merit. Figure of merit of the materials increases in the form of low dimensional structure -nanowire. For the acoustic phonon scattering, thermoelectric behaviour of Silicon nanowire enhances due to the contribution of sub-bands beyond the quantum size limit and multi band effect has play significant role in transport phenomenon. The large value of operating temperature range, low values of thermal conductivity and high value of ZT makes Silicon nanowire useful for thermoelectric materials at high temperature. The high conversion efficiency of thermoelectric chip based on Silicon nanowire can be commercialised used in industry.**

***Keywords*: quantum size limit, nano wire, transport phenomenon, sub-bands.**

1. Introduction

The maximum efficiency is given by $\emptyset_{max} = \eta_c \gamma$ where $\eta_c = \frac{T_H - T_C}{T_H}$ and $\gamma = \frac{\sqrt{1+Z\bar{T}}-1}{\sqrt{1-Z\bar{T}}+\frac{T_C}{T_H}}$ and $\bar{T} = \frac{T_H+T_C}{2}$ .The maximum efficiency is thus the product of the Carnot efficiency and γ which is depends on the parameters of the materials. The concept of a figure-of-merit for a material is employed and given by $Z = \frac{\alpha^2\sigma}{k_e+k_L}$ the term $\alpha^2\sigma$ refers electrical power factor, α Seebeck coefficient, σ electrical conductivity, $k_L$lattice thermal conductivity and k_e electronic thermal conductivity[1-10].The conversion efficiency depends up on operating temperature difference and for a given values of the material's figure-of-merit. The Carnot efficiency is large as temperature differences higher. Although the properties favourable for thermoelectric applications were well known the important advantages offered by semiconductors were overlooked with the attention of researchers focused on metals and metal alloys. In metals the electronic contribution to thermal conductivity is a major contribution. The ratio of electronic thermal conductivity to electrical conductivity is constant (Wideman-Franz Law). In1956 Ioffe and co-workers demonstrated that the ratio of electrical and thermal conductivities could be decreased if the thermoelectric materials are alloyed with an isomorphous element or compound. Spurred on by possible military application a tremendous survey of materials was undertaken, particularly at the RCA laboratories in the USA, which resulted in the discovery of a few semiconductors with significantly higher figure-of-merit. Conventional thermoelectric materials may be divided into four categories depending upon their operating temperature range: Bismuth-antimony alloys, for which useful operating temperature range is100-200K and could be useful in cry-o-electronic devices. Bismuth telluride and it alloys with antimony telluride and bismuth selenide possess high figure-of-merit at around room temperature. Lead telluride and it alloys operate in the intermediate temperature range (500-800K) and are employed in space exploration. Silicon-germanium alloys and TAGS (tellurium – antimony – germanium -silver) have low figure-of-merit around room temperatures but are useful for high temperature (>1000K) applications [10-20]. Silicon is used an excellent material for the fabrication of devices in the microelectronic industry. The silicon nanowires showed a thermal conductivity as small as 2 W/(m K)[11].

2. Figure-of-Merit for Nanowire

The system under investigation in the form of a rectangular silicon nanowire which characterised by transverse dimensions 'a' and 'b' and a wire of length L along the z-axis. The Transport coefficients for such a system are given by such as electrical conductivity, Seebeck coefficient, and the electronic contribution to thermal conductivity given as: [3,5,10]

$$\sigma = \frac{2\tau_0 e^2}{\pi\hbar ab(2m_z^*)^{1/2}} B_6 \quad (1)$$

$$\alpha = \frac{k_B}{e}\left[\frac{E_F}{k_BT} - \frac{B_4+B_5}{k_BTB_6}\right] \quad (2)$$

$$k_e = \left(\frac{k_B}{e}\right)^2 \left[\frac{B_1+2B_2+B_3}{(k_BT)^2B_6} - \left(\frac{B_4+B_5}{k_BTB_6}\right)^2\right] \sigma T \quad (3)$$

where B1, B2, B3, B4, B5, and B6 are given by

$$B_1 = \sum_n \sum_l \left(p+\frac{5}{2}\right)(k_BT)^{\left(p+\frac{5}{2}\right)} F_{\left(p+\frac{3}{2}\right)}(\eta_{n,l}) \quad (4)$$

$$B_2 = \sum_n \sum_l (E_n' + E_l')\left(p+\frac{3}{2}\right)(k_BT)^{\left(p+\frac{5}{2}\right)} F_{\left(p+\frac{1}{2}\right)}(\eta_{n,l}) \quad (5)$$

$$B_3 = \sum_n \sum_l (E_n' + E_l')^2\left(p+\frac{1}{2}\right)(k_BT)^{\left(p+\frac{5}{2}\right)} F_{\left(p-\frac{1}{2}\right)}(\eta_{n,l}) \quad (6)$$

$$B_4 = \sum_n \sum_l \left(p+\frac{3}{2}\right)(k_BT)^{\left(p+\frac{3}{2}\right)} F_{\left(p+\frac{1}{2}\right)}(\eta_{n,l}) \quad (7)$$

$$B_5 = \sum_n \sum_l (E_n' + E_l') \left(p + \frac{1}{2}\right) (k_B T)^{\left(p+\frac{3}{2}\right)} F_{\left(p-\frac{1}{2}\right)}(\eta_{n,l}) \quad (8)$$

$$B_6 = \sum_n \sum_l \left(p + \frac{1}{2}\right) (k_B T)^{\left(p+\frac{1}{2}\right)} F_{\left(p-\frac{1}{2}\right)}(\eta_{n,l}) \quad (9)$$

where $F_{(p)}(\eta_{n,l})$ is Fermi-integral defined as

$$F_{(p)}(\eta_{n,l}) = \int_0^{\infty} \frac{x^p}{\exp(x-\eta_{n,l})+1} dx \quad (10)$$

$E_n' = \frac{E_n}{k_B T}$ $E_l' = \frac{E_l}{k_B T}$, reduced carrier energy $x = \frac{\varepsilon}{k_B T}$ with respect to conduction band edge, $\eta_{n,l} = \xi - E_n' - E_l'$; reduced Fermi energy $\xi = \frac{E_F}{k_B T}$. Here summation taken over several sub-bands.

The relaxation time for acoustic phonon scattering in one-dimensional systems is essentially energy dependent and is given by [19]

$$\tau = \frac{4}{9} \frac{\hbar^2 c_{11} ab}{2\, \varepsilon_1^2 k_B T (2m_Z^*)^{\frac{1}{2}}} \varepsilon^{\frac{1}{2}} \quad (11)$$

In nano wire system due to modification of the phonon group velocities and dispersion are spatial confinement leads to a significant increase of the phonon relaxation rates, therefore a significant drop in the lattice thermal conductivity. As wire diameter decreases enhance surface scattering of phonon thermal conductivity reduced [11,19]

The dimensionless figure of merits is given by

$$ZT = \frac{\alpha^2 \sigma}{k_e + k_L} T$$

3. Results and Discussion

The theoretical model described here has been applied to Silicon nanowire. Figures 1 illustrate the variation of the Seebeck coefficient versus temperature for 100nm silicon nano wire. For the mode (n,m) = (1,1) as temperature increased value of Seebeck coefficient decreased very slowly and at 900 K its value reduced up to 176.2x10^{-6}V/K.

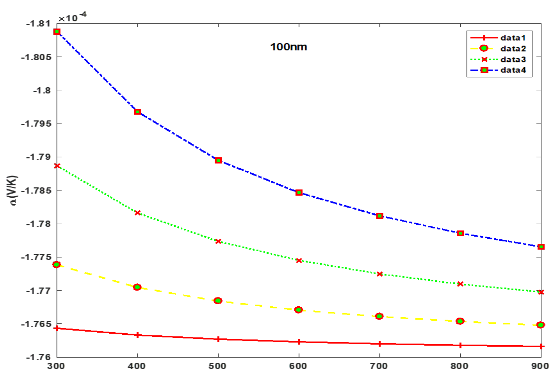

Fig. 1. Variation of Seebeck Coefficient of Si nanowire of 100nm data1 refers mode (n,m) = (1,1) this indicates that all sub-bands below or equal to (1,1) have been considered (+); data2 refers mode (n,m) = (2,2) all sub-bands below or equal to (2,2) have been considered (o); data3 refers mode (n,m) = (3,3) indicates that all sub-bands below or equal to (3,3) have been considered (x);data4 referes mode (n,m) = (4,4) indicates that all sub-bands below or equal to (4,4) have been considered (□).

The mode (n, m) = (2,2) the Seebeck coefficient decreases from 177.4x10^(-6) V/K. fallowed the path like parabola and approach towards the value 176.4x10^(-6) V/K. . Similarly, mode (n, m) = (3,3) asymptotic approach towards the value 177x10^(-6) V/K. And mode (n, m) = (4,4) asymptotic approach towards the value177.7x10^(-6) V/K. The Seebeck coefficient ranges from 176.2 to 180.9 μV/K.

Figures-2. Illustrate the variation of the electronic thermal conductivity versus temperature for 100nm Si nano wire. For the mode (n,m) = (1,1) as temperature increased value of electronic thermal conductivity increased with costant gradient and at 900K it value is $0.04688(W/_{m-K})$. For the mode (n,m) = (2,2) as temperature increased value of electronic thermal conductivity increased with grater gradient as compared to (1 ,1) and at 900K it value is $0.105(W/_{m-K})$. That shows that contribution in electrical conductivity 128 % jumped when the electrons mode (2,2) contributes in transportation. Similarly, mode (n, m) = (3,3) 900K it value is $0.1855(W/_{m-K})$ And mode (n, m) = (4,4) 900K it value is $0.2873(W/_{m-K})$.

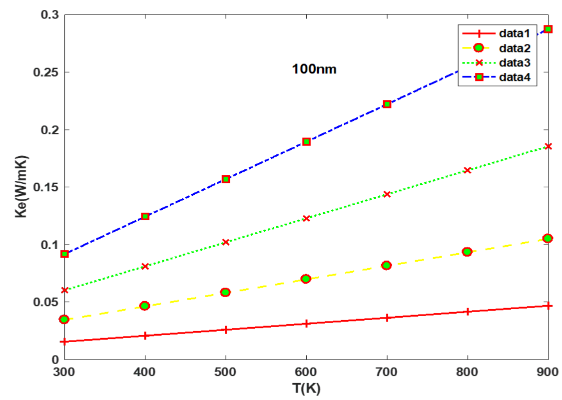

Fig. 2. Variation of electronic contribution of thermal conductivity of Si nanowire of 100nm data1 refers mode (n,m) = (1,1) this indicates that all sub-bands below or equal to (1,1) have been considered (+); data2 refers mode (n,m) = (2,2) all sub-bands below or equal to (2,2) have been considered (o); data3 refers mode (n,m) = (3,3) indicates that all sub-bands below or equal to (3,3) have been considered (x);data4 referes mode (n,m) = (4,4) indicates that all sub-bands below or equal to (4,4) have been considered (□).

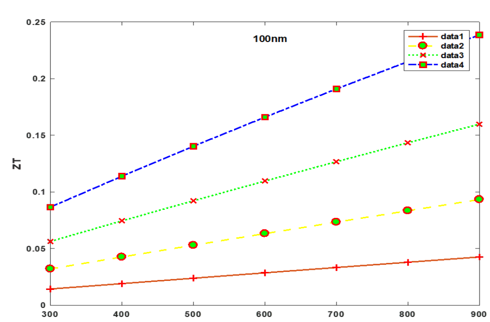

Figure-3.Variation Thermoelectric figure-of merits ZT of Si nanowire of 100nm data1 refers mode (n,m) = (1,1) this indicates that all sub-bands below or equal to (1,1) have been considered (+); data2 refers mode (n,m) = (2,2) all sub-bands below or equal to (2,2) have been considered (o); data3 refers mode (n,m) = (3,3) indicates that all sub-bands below or equal to (3,3) have been considered (x);data4 referes mode (n,m) = (4,4) indicates that all sub-bands below or equal to (4,4) have been considered (□).

Figures-3 illustrate the variation of the dimensionless figure-of-merits ZT versus temperature for 100nm Si nano wire optimum reduced fermi energy 0.5. As temperature increased value of ZT increased monotonically and at high temperature asymptotic approach towards the value 0.04 .The mode (n, m) = (2,2) the ZT fallowed the path like parabola at high temperature asymptotic approach towards the value 0.093 That shows that contribution in ZT 132 % jumped when the electrons mode (2,2) contributes in transportation. Similarly, mode (n, m) = (3,3) asymptotic approach towards the value 0.1599. And mode (n, m) = (4,4) asymptotic approach towards the value 0.2386.

The large value of operating temperature range, low values of thermal conductivity and high value of ZT makes Silicon nanowire useful for thermoelectric materials at high temperature. Due to high conversion efficiency thermoelectric chip based on Silicon nanowire may be commercialised used in industry.

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