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THERMOELECTRIC COEFFICIENTS OF HEAVILY DOPED N-TYPE SILICON[†]

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In this study the thermoelectric effect is investigated in terms of thermoelectric power, Figure of merit(ZT), and power factor. The calculations were carried out based on Boltzmann transport equation by taking ionized impurity scattering as a dominant mechanism for heavily doped n-type silicon at 300K with charge concentration varies from 2×10^{18} /cm^3 – 20×10^{20} /cm^3. It is known that doping of materials can induce Fermi level shifts and doping can also induce changes of the transport mechanisms. The result of this study shows doping also induces changes in thermoelectric power, Figure of merit, and power factor. The magnitude of the change is different for consideration of parabolic density of states and non-parabolic modified density of states which amounts to 16.7% for thermoelectric power, from 0.059% - 84.1% for Figure of merit(ZT) in favor of non-parabolic consideration respectively. There is also a difference of 39.9% for power factor with respect to relaxation time between the two cases in favor of the parabolic consideration.

Key words: doping, thermoelectric effect, thermoelectric power
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A semiconductor can be considered heavily doped when the impurity band associated with the doped impurity merges with either in the conduction and valence band. There are two aspects with direct influence on the carrier transport namely tailing of states into the band gap. It thus seems useful to determine theoretically the location of the Fermi level in heavily doped silicon taking into account the density of states in the tails [1-3]. According to [1], the density of state for heavily doped silicon is expressed in [4] as

$$\rho(z) = \frac{m_b^{*\frac{3}{2}} 2^{\frac{3}{4}} \delta^{\frac{1}{2}}}{\pi^2 \hbar^3} y(z) \tag{1}$$

whereas,

$$\rho(\mathrm{E}) = \frac{8\sqrt{2}\pi m_n^{*\frac{3}{2}}}{h^3} E^{\frac{1}{2}} \tag{2}$$

represents the parabolic total density of states in the conduction band.

In Eq. (1) for non-parabolic modified density of states, the term y(z) is given by

$$y(z) = \frac{1}{2}\int_{-\infty}^{z} (z-\zeta)^{\frac{1}{2}} \exp(-\zeta^2) d\zeta \tag{3}$$

and

$$z = \frac{E}{\sqrt{2}\delta} \tag{4}$$

The standard deviation of the Gaussian distribution for the impurity potential energy is

$$\delta = \left(\frac{n e^4 a_s}{8\pi\epsilon_0^2\epsilon_d^2}\right)^{\frac{1}{2}} = \left(\frac{N_d e^4 a_s}{8\pi\epsilon_0^2\epsilon_d^2}\right)^{\frac{1}{2}} \tag{5}$$

For a screened coulomb potential of impurity atoms with ϵ_d is the dielectric constant of the given semiconductor. The Thomas-Fermi screening length according to [5] is

$$a_s = \left(\frac{\pi^{\frac{4}{3}}\epsilon_0\epsilon_d\hbar^2}{3^{\frac{1}{3}} N_d^{\frac{1}{3}} e^2 m_n^*}\right)^{\frac{1}{2}} \tag{6}$$

The density of states function given by Eq. 1 is very complicated and thus is not useful for making any calculation. Slotboom [2] has however; suggested the following approximation for y(z).

$$y(z) \cong z^{\frac{1}{2}}\left[1 - \frac{1}{16z^2}\right] \tag{7}$$

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for z > 0.601, equally, E > 0.85δ.
and

$$y(z) \cong \frac{1}{2\pi^{\frac{1}{2}}}\exp(-z^2)\{1.225 - 0.906[1 - \exp(2z)]\} \tag{8}$$

for z ≤ 0.601.

Using Eqs. (7) and (8) for y(z), we obtain the following expression of the electron concentration in the conduction band for modified density of states having band tails

$$n = 2\int f_0\,\rho(E)dE = \frac{m_n^{*\frac{3}{2}}2^{\frac{5}{4}}\delta^{\frac{3}{2}}}{\pi^2\hbar^3}\psi_0 \tag{9}$$

where ψ_0 is obtained by setting λ = 0 into

$$\psi_\lambda = \frac{1}{2\pi^{\frac{1}{2}}}\int_{-\infty}^{0.601}|z|^\lambda \exp(-z^2)\left(\frac{0.319+0.906\mathrm{Exp}(2z)}{1+\mathrm{Exp}\left\{1.494n_n^{\frac{5}{12}}z-\eta\right\}}\right)dz + \int_{0.601}^{\infty}\frac{z^{\frac{1}{2}}\left[1-\frac{1}{16z^2}\right]}{1+\exp\left\{1.494n_n^{\frac{5}{12}}z-\eta\right\}}dz \tag{10}$$

It is more convenient to introduce normalized electron concentration n_n given by

$$n_n = \frac{n}{10^{25}/m^3} \tag{11}$$

In this study the semi-classical and quantum treatments are applied in the calculations of scattering mechanisms under the assumptions of the electron concentrations from 2×10^{18} - $2\times10^{20}/cm^3$ and in the temperature range 77 – 300K.

LINEARIZED BOLTZMANN EQUATION WITH RELATION TIME APPROXIMATION

All the quantities of interest to us may be expressed immediately in terms of Fermi-Dirac distribution f(**r**,**k**.t). The Boltzmann transport equation is therefore

$$\frac{\partial f}{\partial t} + \mathbf{v}.\nabla f + \mathbf{F}.\nabla_{\mathbf{k}} f = \left(\frac{\partial f}{\partial t}\right)_{\mathbf{c}} \tag{12}$$

Consider a time dependent but spatially homogenous situation in the absence of applied fields. Thus Eq. (12) becomes

$$\frac{\partial f}{\partial t} = \left(\frac{\partial f}{\partial t}\right)_c \tag{13}$$

where the term $\left(\frac{\partial f}{\partial t}\right)_c$ is expressed in terms of collision operator **C** as

$$\left(\frac{\partial f}{\partial t}\right)_c = \boldsymbol{C}\phi(\boldsymbol{r},\boldsymbol{k}) = \beta\int V(\boldsymbol{k}',\boldsymbol{k})[\phi(\boldsymbol{k}') - \phi(\boldsymbol{k})]\boldsymbol{dk} \tag{14}$$

for arbitrary function(ϕ) and potential(V). In the relaxation time approximation, we suppose that $\left(\frac{\partial f}{\partial t}\right)_c$ has the simplest form which will yield the behavior

$$\left(\frac{\partial f}{\partial t}\right)_c = -\frac{f(K)}{\tau} \tag{15}$$

Now for all mechanisms of interest to us, E is not much changed in a single event. For elastic scattering such as ionized impurity scattering this is strictly true, while for acoustic deformation potential scattering(through local band perturbation), it is only approximate. Actually in the cases for which τ is well defined, it is a function of E alone. Thus the relaxation time can be written as

$$\tau = \tau_0 E^\lambda \tag{16}$$

The value of the superscript λ depends on the scattering mechanism 3/2 for ionized mpurities and -1/2 for acoustic phonons. In the case of optical phonons the electron scattering is not elastic the relaxation time cannot be applied [6].

ELECTRON AND HEAT FLUX DENSITIES

In the steady state in a homogeneous system with electric E applied along the x-axis, in the absence of magnetic field, the distribution can be written as

$$f = f_0 + f' \tag{17}$$

which is the solution of

$$-\frac{e}{\hbar}\boldsymbol{E'}.\boldsymbol{\nabla}_{\mathbf{k}}\mathrm{f}_0 = \left(\frac{\partial f'}{\partial t}\right)_{\mathrm{coll}} \tag{18}$$

where f_0 is the thermal equilibrium distribution and f' is a first order perturbation given by

$$f' = v_x f_x + v_y f_y + v_z f_z \tag{19}$$

Furthermore,

$$v\left(-\frac{\partial f}{\partial E}\right) = -\frac{1}{\hbar}\frac{\partial f}{\partial k} \tag{20}$$

And Eq. (18) can be solved to find f_x for one-dimensional case using Eqs. (15), (19), and (20) to give

$$f_x = \tau e\left(\frac{\partial f_0}{\partial E}\right)E'_x \tag{21}$$

Since E'_x in Eq. (21) is the d.c. electric field along x-direction, and the x-component of the electric current density is given by

$$J_x = -\frac{2em_n^{*3}}{\hbar^3}\int v_x^2 f_x dv_x dv_y dv_z \tag{22}$$

Finally after transformation to spherical coordinates (v, θ, φ) for velocity components and making use of Eq. (21) for f_x , we get

$$J = -\frac{e^2 m_n^{*3} E' v_0^5}{6\pi^2\hbar^3}\int_0^\infty \tau(E)\frac{\partial f_0}{\partial E}\varepsilon^{\frac{3}{2}}d\varepsilon \tag{23}$$

where we make change of variable from v to $\varepsilon = E/k_B T$.

Thus for the case of parabolic density of states we obtain the following expression for the electrical conductivity

$$\sigma = \frac{2ne^2\tau_0}{m_n^*}\frac{\int_0^\infty \varepsilon^2 f_0 d\varepsilon}{\int_0^\infty \varepsilon^{\frac{1}{2}} f_0 d\varepsilon} = \frac{2ne^2\tau_0}{m_n^*}\frac{F_2}{F_{\frac{1}{2}}} \tag{24}$$

where $F_{1/2}$ and F_2 can obtained as family of the well known tabulated Fermi-integral by setting p equals to 3 and 4 respectively.

$$\int_0^\infty \frac{\varepsilon^p d\varepsilon}{1+\exp(\varepsilon-\eta)} \tag{25}$$

where $\eta = E_F/k_B T$ is normalized Fermi energy.

We can obtain similar expression for electrical conductivity for the case of non-parabolic modified density of states having band tails in Eq. (1) by inserting into Eq. (24) which gives

$$\sigma = \frac{2e^2 n\tau_0}{3m_n^*}\left(\frac{\sqrt{2}\delta}{k_B T}\right)^{\frac{5}{2}}\frac{\psi_{\frac{5}{2}}}{\psi_0} \tag{26}$$

where $\psi_{\frac{5}{2}}$ is obtained from Eq. (10) by setting $\lambda = 5/2$.

To obtain thermal current density, we use from[7,8]

$$Q_x = \frac{2m_n^{*3}}{h^3}\int\left(\frac{1}{2}m_n^* v^2\right)v_x f d^3v = \frac{-4\pi m_n^{*4}}{5\hbar^4}\int_0^\infty v^6 f_x dv \tag{27}$$

after integrating over spherical coordinates θ and φ.

In the presence of an external d.c. field E'_x and a temperature gradient dT/dx along the x-direction, the Boltzmann transport equation is written as

$$v_x\frac{\partial f_0}{\partial x} - \frac{eE'_x}{m_n^*}\frac{\partial f_0}{\partial v_x} = v_x\frac{\partial f_0}{\partial x} - \frac{eE'_x}{m_n^*}\frac{v_x}{v}\frac{\partial f_0}{\partial v} = -\frac{f-f_0}{\tau} = -\frac{v_x f_x}{\tau} \tag{28}$$

One can solve $\frac{\partial f_0}{\partial x}$ in Eq. (28) as

$$\frac{\partial f_0}{\partial x} = \frac{\partial f_0}{\partial T}\frac{\partial T}{\partial x}$$

$$= \left(-\frac{\partial f_0}{\partial E}\right)\left[\frac{E}{T} + k_B T\frac{\partial}{\partial T}\left(\frac{E_F}{k_B T}\right)\right]\left(\frac{dT}{dx}\right) \tag{29}$$

Inserting Eq. (29) into Eq. (28) and solving for f_x, we get

$$f_x = \tau\frac{dT}{dx}\frac{\partial f_0}{\partial E}\left[\frac{E}{T} + k_BT\frac{\partial}{\partial T}\left(\frac{E_F}{k_BT}\right)\right] + eE_x'\tau\frac{\partial f_0}{\partial E} \tag{30}$$

Substituting Eq. (30) into Eq. (23), J_x becomes

$$J_x = -\frac{em_n^{*3}}{3\pi^2\hbar^3}\int_0^\infty \tau v^4\frac{\partial f_0}{\partial E}\left[\frac{E}{T} + k_BT\frac{\partial}{\partial T}\left(\frac{E_F}{k_BT}\right)\right]\left(\frac{dT}{dx}\right)dv - \frac{e^4m_n^{*3}E_x'}{3\pi^2\hbar^3}\int_0^\infty \tau v^4\frac{\partial f_0}{\partial E}dv \tag{31}$$

Since a small current flows, $J_x = 0$ is assumed for measured thermoelectric voltages(V), and we obtain the following relationship between E‘$_x$ and dT/dx.

$$E_x' = -\left(\frac{dT}{dx}\right)\frac{\left[\int_0^\infty \tau v^4\left(-\frac{\partial f_0}{\partial E}\right)\frac{E}{T}dv + \int_0^\infty \tau v^4\left(-\frac{\partial f_0}{\partial E}\right)k_BT\frac{\partial}{\partial T}\left(\frac{E_F}{k_BT}\right)\right]dv}{e\int_0^\infty \tau v^4\left(-\frac{\partial f_0}{\partial E}\right)dv} \tag{32}$$

If there are no gradients of concentration, then the second term in numerator is cancelled. The Seebeck coefficient(α) referred to as the thermal emf or thermoelectric power [9] is given by

$$\alpha = \frac{dV}{dT} = -\frac{1}{eT}\frac{\int_0^\infty \tau v^4\left(-\frac{\partial f_0}{\partial \varepsilon}\right)\frac{E}{T}dv}{\int_0^\infty \tau v^4\left(-\frac{\partial f_0}{\partial E}\right)dv} = -\frac{1}{eT}\frac{\int_0^\infty E^4f_0dE}{\int_0^\infty E^3f_0dE} = -\frac{k_B}{e}\frac{\int_0^\infty \varepsilon^4f_0d\varepsilon}{\int_0^\infty \varepsilon^3f_0d\varepsilon} = -\frac{k_B}{e}\frac{F_4}{F_3} \tag{33}$$

According to [10] dimensionless figure-of-merit(ZT) for a material in terms of Seebeck coefficient(α) , electrical conductivity (σ), and the electronic thermal conductivity (K_e) is

$$ZT = \frac{\alpha^2\sigma T}{K_e} = \frac{\left(-\frac{k_BF_4}{eF_3}\right)^2\left(\frac{2ne^2\tau_0F_2}{m_n^*F_{\frac{1}{2}}}\right)T}{\left(\frac{2n\tau_0(k_BT)^2}{m_n^*T}\left[\frac{10F_4}{3F_{\frac{1}{2}}} - \frac{32}{9}\frac{F_3^2}{F_{\frac{1}{2}}F_2}\right]\right)} = \frac{1}{T}\left[\frac{10}{3}\frac{F_3^2}{F_2F_4} - \frac{32}{9}\frac{F_3^4}{F_2^2F_4^2}\right]^{-1} \tag{34}$$

The power factor (P_{FF}) for the case of parabolic density of state is

$$P_{FF} = \alpha^2\sigma = \left(-\frac{k_B}{e}\frac{F_4}{F_3}\right)^2\left(\frac{2ne^2\tau_0}{m_n^*}\frac{F_2}{F_{\frac{1}{2}}}\right) = \frac{2nk_B^2\tau_0}{m_n^*}\frac{F_4^2F_2}{F_3^2F_{1/2}} \tag{35}$$

where F_3 and F_4 can obtained as family of the well known tabulated Fermi-integral by setting p equals to 3 and 4 respectively.

We can obtain expressions for α, ZT and P_{FF} for the case of modified density of states using the corresponding expressions, i.e., Eqs. (33-35) obtained based on standard model with parabolic density of states (which doesn't incorporate the effect of band tails) by substituting Eq. (1) for modified density of states and by extending the integration limits from -∞ to ∞. This yields the following expressions

$$\alpha = -\frac{\sqrt{2}\delta}{eT}\frac{\psi_{7/2}}{\psi_{5/2}} \tag{36}$$

and

$$ZT = \frac{\alpha^2\sigma T}{K_e} = \frac{\left(-\frac{\sqrt{2}\delta^{\psi_{7/2}}}{eT\,\psi_{5/2}}\right)^2\left(\frac{2e^2n\tau_0}{3m_n^*}\left(\frac{\sqrt{2}\delta}{k_BT}\right)^{\frac{5}{2}}\frac{\psi_{\frac{5}{2}}}{\psi_0}\right)}{\frac{2n\tau_0(k_BT)^2}{3m_n^*T}\left(\frac{\sqrt{2}\delta}{k_BT}\right)^{\frac{9}{2}}\left[\frac{\psi_{\frac{9}{2}}}{\psi_0} - \frac{\psi_{\frac{7}{2}}^2}{\psi_0\psi_{\frac{5}{2}}}\right]} = \frac{1}{T}\left[\frac{\psi_{\frac{5}{2}}\psi_{\frac{9}{2}}}{\psi_{\frac{7}{2}}^2} - 1\right]^{-1} \tag{37}$$

Finally

$$P_{FF} = \left(-\frac{\sqrt{2}\delta}{eT}\frac{\psi_{7/2}}{\psi_{5/2}}\right)^2\left(\frac{2e^2n\tau_0}{3m_n^*}\left(\frac{\sqrt{2}\delta}{k_BT}\right)^{\frac{5}{2}}\frac{\psi_{\frac{5}{2}}}{\psi_0}\right) = \frac{2n\tau_0\left(\frac{\sqrt{2}\delta}{T}\right)^{\frac{9}{2}}}{3m_n^*k_B^{\frac{5}{2}}}\frac{\psi_{7/2}^2}{\psi_{5/2}\psi_0} \tag{38}$$

where $\psi_{5/2}$, $\psi_{7/2}$, $\psi_{9/2}$ are obtained from Eq. (10) by setting λ = 5/2, 7/2, 9/2 respectively.

RESULTS

Thomas-Fermi screening length in Eq.(6) is calculated to be

$$a_s = 7.87X10^{-10}n_n^{-\frac{1}{6}}\,m \tag{39}$$

and the value of the Gaussian distribution for impurity potential energy is

$$\delta = 4.375\,X10^{-21}n_n^{\frac{5}{12}}J \tag{40}$$

Thus the electron concentration in the conduction band for modified density of states having band tails in Eq. (9) becomes

$$n = \frac{m_n^{*\frac{3}{2}} 2^{\frac{5}{4}}}{\pi^2 \hbar^3} \frac{1}{2\pi^{\frac{1}{2}}} \int_{-\infty}^{0.601} \delta^{\frac{3}{2}} exp(-z^2) \left(\frac{0.319+0.906exp(2z)}{1+exp\left\{1.494 n_n^{\frac{5}{12}} z-\eta\right\}} \right) dz + \int_{0.601}^{\infty} \frac{\delta^{\frac{3}{2}} z^{\frac{1}{2}} \left[1-\frac{1}{16z^2}\right]}{1+exp\left\{1.49 n_b^{\frac{5}{12}} z-\eta\right\}} dz$$

$$= \frac{(1.18)^{\frac{3}{2}} X (9.11)^{\frac{3}{2}} X (10^{-31})^{\frac{3}{2}} X 2^{\frac{5}{4}} X (4.375)^{\frac{3}{2}} X (10^{-21})^{\frac{3}{2}} (0.3)^{\frac{5}{8}}}{\pi^2 X (1.054)^3 X 10^{-102}}$$

$$[\int_{-\infty}^{0.601} (0.28) exp(-z^2) \left(\frac{0.319+0.906exp(2z)}{1+exp\{1.494X0.603z-\eta\}} \right) dz + \int_{0.601}^{\infty} \frac{z^{\frac{1}{2}}\left[1-\frac{1}{16z^2}\right]}{1+exp\{1.49X0.603z-\eta\}} dz\ ] = 3.2X10^{25}\mathrm{X}$$

$$[\int_{-\infty}^{0.601} (0.28) exp(-z^2) \left(\frac{0.319+0.906exp(2z)}{1+exp\{0.9z-\eta\}} \right) dz + \int_{0.601}^{\infty} \frac{z^{\frac{1}{2}}\left[1-\frac{1}{16z^2}\right]}{1+exp\{0.9z-\eta\}} dz\ ] \tag{41}$$

Thus

$$n_n = 3.2[\int_{-\infty}^{0.601} (0.28) exp(-z^2) \left(\frac{0.319+0.906exp(2z)}{1+exp\{0.9z-\eta\}} \right) dz + \int_{0.601}^{\infty} \frac{z^{\frac{1}{2}}\left[1-\frac{1}{16z^2}\right]}{1+exp\{0.9z-\eta\}} dz\ ] \tag{42}$$

Similarly for parabolic density of states

$$\mathrm{n_n} = 3.2\mathrm{F}_{1/2}(\eta) \tag{43}$$

and the rest all integrals are evaluated by inserting them directly in the mathematical v.5 installed in the sun ultra 5 work station computer[11]. The above values of n_n and η obtained by an iterative method which was employed in the above simplified expressions to relate them for parabolic and modified density of states cases.
The table of values(in the Appendix part of Table 1 and 2), $F_{1/2}$ (-2.6) is evaluated as

$$\mathrm{NIntegrate}\left[x^{1/2}/(1+\mathrm{Exp}[x+2.6])\ /\right], \{x, 0, \infty\}$$

The result is $F_{1/2}$ (-2.6) = 0.0641614 and the corresponding normalized concentration is

n_n = 3.2 $F_{1/2}$(-2.6) = 3.2*0,0641614 = 0.2048

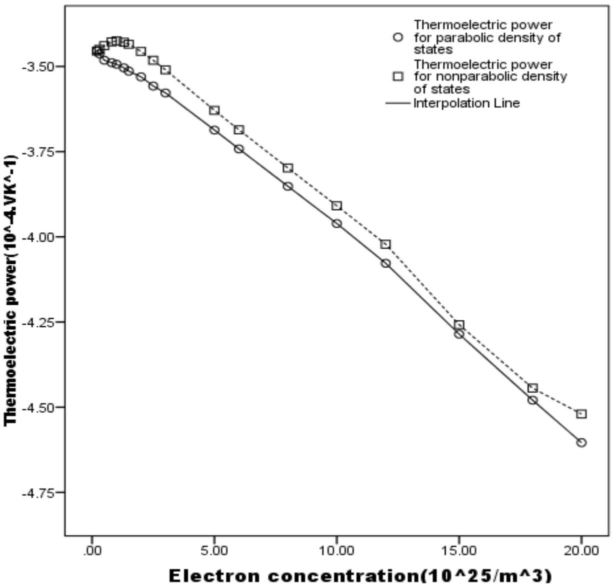

Figure 1. Thermoelectric power as a function of electron concentration with the solid line marked by circles is for parabolic band and dashed line marked by squares is for modified density of states.

Note that iterative method is not one shot process but it takes certain thoughtful steps to get the best value of η which gives to the nearest possible value of n_n = 0.2 that is η = -2.6. This procedure was followed to evaluate all values in the table including the corresponding values for F_3, and F_4 for parabolic case.

It is straightforward to use the same procedure for the case of modified density of states. In the same way as the previous case, in the table of values, n_n = 0.2 corresponds to η = -2.9. Mathematica software 5.0 is used to obtain 0.0333945 + 0.13557 = 0.16896 which was taken as the best approximation of n_n = 0.2 during the iterating method corresponding to η = -2.9. The same procedure was used for the other pair of values in the table. The values of the other integrals ψ_0 , $\psi_{\frac{5}{2}}$, $\psi_{\frac{7}{2}}$, $\psi_{\frac{9}{2}}$ (in Appendix part of Table 2) were evaluated straight forward(even copy and paste of expressions is possible that facilitates the process) by using mathematica v.5.

Graph in Figure 1 represents the dependence of thermoelectric power, defined as the voltage difference (ΔV) developed due to temperature difference (ΔT), as a function of electron concentration ranging 0.2 – 20×10^{25}/m^3 for two different cases. The quadratic equation fitting results are given by y = -0.006x^2 + 0.06x -3.584 and with goodness of fit R^2 = 0.987 for parabolic case whereas y = $-0.007x^2 + 0.072x - 3.577$ and with goodness of fit $R^2 = 0.99$ for non-parabolic case. When we compare the quadratic terms for each case the corresponding coefficients -0.007 and -0.006 differ by (-0.006 + 0.007)/0.006 = 16.7%, the coefficients of the linear terms differ by (0.072 -0.06)/0.06 = 16.7%, and the difference b/n the constant terms is negligible. Thus the values of the seebeck coefficient differ by 16.7% in favor of non-parabolic density of states consideration.

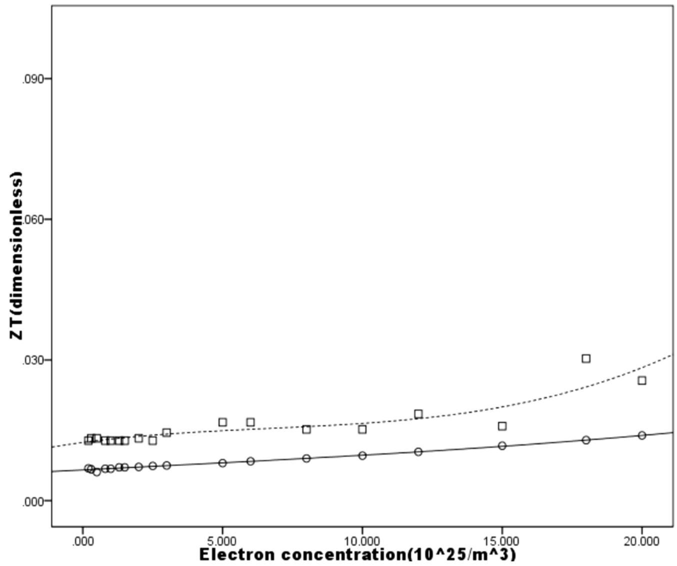

Figure 2. Merit(ZT) as a function of electron concentration with the solid line marked by circles is for parabolic band and dashed line marked by squares is for non-parabolic band consideration.

The graph for values of Figure of merit (ZT) for both parabolic and non-parabolic cases are presented in Figure 2. The cubic curve fitting was used with $R^2 = 0.994$ for parabolic case and $R^2 = 0.814$ for non-parabolic case. The maximum value of ZT for parabolic case is 0.0139 and for non-parabolic case it is 0.0256 corresponding to the maximum carrier concentration of 2 X $10^{26}/m^3$. The minimum value of ZT for parabolic case is 0.0069 and for the non-parabolic case it is 0.0128 corresponding to the minimum carrier concentration of $2X10^{24}/m^3$. The difference in the values of ZT ranges up to 0.59% - 84.1% in favor of the non-parabolic consideration.

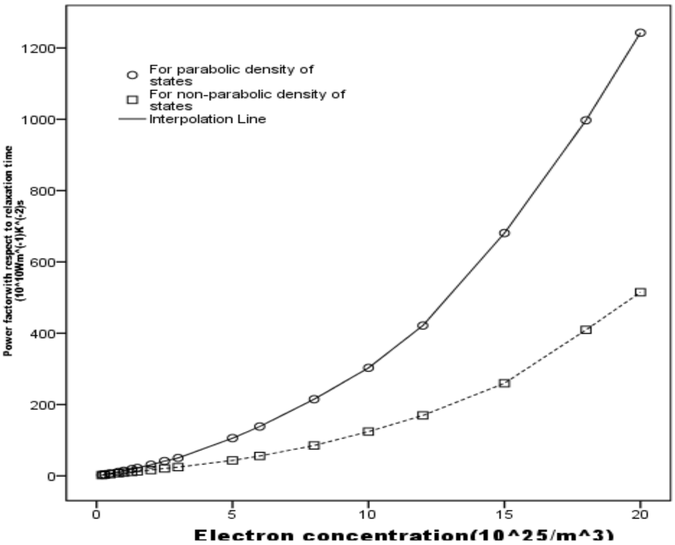

Figure 3. Power factor with respect to relaxation time plotted as a function of electron concentration

The power factor per relaxation time is plotted as shown in Figure 3. An exponential curve fitting is performed for the calculated data to obtain $y = 2.059e^{0.355x}$ and with goodness of fit $R^2 = 0.993$ for parabolic case while $y = 1.66e^{0.307x}$ and with goodness of fit $R^2 = 0.987$ is obtained for non-parabolic case. The two curves differ as shown by the respective exponential functions as the first is growing by a factor of 0.355 while the second is growing by a factor of 0.307 with a difference of .2% in favor of the non-parabolic consideration. On the other hand the amplitudes of the exponential functions are 2.059 for the first case and 1.66 for the second case which differ by 39.9% in favor of the parabolic consideration.

The results about calculations of Seebeck coefficient(α), Figure of merit(ZT), and Power factor with respect to relaxation time(P_{FF}/τ_0) for the parabolic and non-parabolic considerations do differ as much as 16.7%, from 0.059% to 84.1%, 39.9% respectively. The magnitude of the difference 16.7% is obtained in favor of parabolic density of states consideration as compared to non-parabolic density of states. It tells us as the carrier concentration increases with incorporation of more impurities the Seebeck coefficient changes significantly in both cases with respective difference of 16.7%. This is evident in the pattern of the calculated data fitted with a quadratic curve where the good-of-fit has a maximum value than other curves. When it comes to the Figure-of-merit(ZT) the maximum value of goodness-of-fit of the calculated data is obtained for cubic curve as shown in Figure 2. The comparison is made between the respective values of ZT at the minimum and maximum carrier concentration which gives the difference that ranges from 0.059% - 84.1% where the gap between the values in the two cases increases as the carrier concentration increases. The calculation of the power factor with respect to relaxation time is compared for the two cases with help of an exponential curve fitting which has a maximum value of goodness-of-fit than other fitted curves. Therefore the calculations for the two cases differ as much as 39.9% in favor of the parabolic density of states. This result reminds care should be taken in our calculation of thermoelectric coefficients for higher carrier concentrations where non-parabolic density of states consideration is preferable.

The experimental work by [12] reported that, despite limited information available about thermoelectric properties of single crystal silicon for higher doping concentration at higher temperature, they measured electrical conductivity, Seeback coefficient, and thermal conductivity to get calculated value of ZT as much as 0.015 for n-type silicon and 0.008 for p-type silicon in the heavily doping range(10^{18} – 10^{20}/cm^3) at temperature range from 300 – 1000K. In the current study the maximum value is 0.0256 slightly different by 1.06% from the experimental value for the non-parabolic density of consideration as it is closer than the parabolic consideration which differs as much as 12.4% from the experimental value. Thermoelectric devices provide cooling when an applied current pumps heat from the cold side towards the hot side through the Peltier effect, or enable waste heat recovery by converting a heat gradient to electrical power through the Seebeck effect[13]. As cited in [13], a good thermoelectric material should possess a large Seebeck coefficient, a high electrical conductivity, and low thermal conductivity to maximize the dimensionless Figure of merit for the thermoelectric performance of a material. Reducing the thermal conductivity is therefore a natural way to improve the performance(indicated by power factor and efficiency) of a thermoelectric material. [13] found that the thermal conductivity is strongly reduced due to nanostructuration and the incorporation of impurities.

CONCLUSION

The thermoelectric effect is investigated in terms of thermoelectric power, Figure of merit, and power factor which have primary importance in device application. There is considerable difference of 16.7% between calculated value of thermoelectric power based on the parabolic density of states and the modified density of states in favor of the latter case. The difference between Figure of merit values calculated for two cases ranges from 0.059% - 84.1%% in favor of the non-parabolic case. The same trend is expected for the electron concentration exceeding $2\text{x}10^{26}$/m^3. The calculated values of the power factor with respect to the relaxation time differ between the two case by 39.9% in favor of parabolic consideration. Laws of modern physics are used in the derivation of modified non-parabolic density of states to make corrections for parabolic density of states consideration as applied for heavily doped silicon, by doing so we get significant agreement with experimental results.

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APPENDIX

Table 1. Calculated values for parabolic density of states

Serial No	n_n	η	$F_{1/2}$	F_2	F_3	F_4	$\alpha(\times10^{-4}\ VK^{-1})$	ZT	$P_{FF}/\tau_0(10^{10}W\cdot m^{-1}\cdot K^{-2}\cdot s^{-1})$
1	0.2	-2.6	0.064	0.147	0.444	1.778	-3.4539	0.0069	2.607564
2	0.3	-2.2	0.095	0.22	0.66	2.65	-3.4631	0.0067	3.964446
3	0.5	-1.7	0.15	0.37	1.08	4.36	-3.4819	0.0061	7.1154
4	0.8	-1.2	0.24	0.58	1.77	7.16	-3.489	0.0068	11.20056
5	1	-0.9	0.32	0.78	2.38	9.64	-3.4935	0.0068	14.15646
6	1.3	-0.6	0.41	1.03	3.19	12.96	-3.5041	0.0071	19.08449
7	1.5	-0.5	0.445	1.13	3.51	14.3	-3.5139	0.0071	22.38165
8	2	-0.1	0.626	1.65	5.17	21.163	-3.5306	0.0072	31.27236
9	2.5	0.2	0.781	2.16	6.87	28.337	-3.5576	0.0074	41.63925
10	3	0.4	0.94	2.583	8.288	34.38	-3.5778	0.0075	50.21136
11	5	1.2	1.56	5.105	17.214	73.58	-3.6867	0.008	105.8283
12	6	1.5	1.875	6.494	22.41	97.230	-3.7421	0.0084	138.4848
13	8	2	2.5	9.513	34.3	153.18	-3.8518	0.009	214.9205
14	10	2.4	3.125	12.68	47.5	218.15	-3.9611	0.0096	302.9532
15	12	2.8	3.75	16.65	65.06	307.59	-4.0777	0.0104	421.5715
16	15	3.4	4.688	24.35	101.6	504.83	-4.2856	0.0117	680.95
17	18	3.9	5.625	32.64	144.13	748.52	-4.4793	0.0129	997.218
18	20	4.2	6.25	38.5	176.12	940.14	-4.604	0.0139	1242.752

Table 2. Calculated values for modified density of states having band tails

Serial No	n_n	η	ψ_0	$\psi_{5/2}$	$\psi_{7/2}$	$\psi_{9/2}$	$\alpha(\times10^{-4}\ VK^{-1})$	ZT	$P_{FF}/\tau_0(10^{10}W\cdot m^{-1}\cdot K^{-2}\cdot s^{-1})$
1	0.2	-2.9	0.08	0..9627	5.047	33.1	-3.455	0.0128	2.32
2	0.3	-2.57	0.09	0.6821	3.015	16.7	-3.45	0.0133	3.35
3	0.5	-2.09	0.12	0.472	1.6809	7.5	-3.439	0.0133	4.9
4	0.8	-1.69	0.14	0.3227	0.9416	3.46	-3.428	0.0128	7.44
5	1	-1.5	0.15	0.2681	0.7124	2.38	-3.425	0.0128	9.09
6	1.3	-1.28	0.17	0.2167	0.5167	1.55	-3.429	0.0128	11.1
7	1.5	-1.15	0.18	0.1933	0.4351	1.23	-3.435	0.0128	12.57
8	2	-0.89	0.2	0.1533	0.3079	0.77	-3.456	0.0133	16.3
9	2.5	-0.68	0.21	0.1287	0.2373	0.55	-3.482	0.0128	20.87
10	3	-0.49	0.23	0.1125	0.1938	0.41	-3.51	0.0145	24.57
11	5	0.1	0.28	0.0803	0.1156	0.20	-3.629	0.0167	43.4
12	6	0.34	0.3	0.0726	0.0984	0.16	-3.686	0.0167	55.94
13	8	0.77	0.33	0.0642	0.0795	0.12	-3.798	0.0152	85.28
14	10	1.16	0.36	0.0606	0.0704	0.1	-3.909	0.0152	124.18
15	12	1.52	0.39	0.0592	0.0656	0.086	-4.022	0.0185	169.64
16	15	2.0	0.42	0.058	0.062	0.08	-4.258	0.0159	259.83
17	18	2.46	0.45	0.059	0.061	0.07	-4.444	0.0303	409.6
18	20	2.74	0.47	0.0604	0.0608	0.069	-4.520	0.0256	514.98

ТЕРМОЕЛЕКТРИЧНІ КОЕФІЦІЕНТИ СИЛЬНО ЛЕГОВАНОГО КРЕМНІЮ N-ТИПУ

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Досліджено термоелектричний ефект з точки зору термоелектричної потужності, добротності (ZT) і коефіцієнта потужності. Розрахунки проводили на основі рівняння переносу Больцмана, взявши іонізоване розсіювання домішок як домінуючий механізм для сильно легованого кремнію n-типу при 300 K з концентрацією заряду від 2×10^{18}/см^3 – 20×10^{20}/см^3. Відомо, що легування матеріалів може викликати зміщення рівня Фермі, а легування також може викликати зміни транспортних механізмів. Результати цього дослідження показують, що легування також викликає зміни термоелектричної потужності, добротності та коефіцієнта потужності. Величина зміни різна для врахування параболічної щільності станів і непараболічної модифікованої щільності станів, яка становить 16,7% для термоелектричної енергії, від 0,059% - 84,1% для показника якості (ZT) на користь непараболічної відповідно. Існує також різниця в 39,9% для коефіцієнта потужності щодо часу релаксації між двома випадками на користь параболічного розгляду.

Ключові слова: легування, термоелектричний ефект, термоелектрична енергія