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PHONON CONDUCTION IN HEAVILY DOPED N-TYPE SILICON

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In n-type semiconductors, if the donor concentration $N_{\mathrm{ex}} > N_{\mathrm{c}}$, the critical concentration of donors, the sample becomes metal. The expression for electron–phonon relaxation rate in such semiconductors in the self-consistent method derived by T. Sota and K. Suzuki, modified in the recent paper of M. K. Roy, is used to take into account a realistic picture of the scattered phonons in heavily doped n-type silicon. Angular average of the deformation potential for different polarization vectors λ obtained by introducing spherical polar coordinates has been used. Finally, we have calculated phonon conductivity K for As- and P-doped silicon with $N_{\mathrm{ex}} > N_{\mathrm{c}}$. Good agreement with the experimental result of M. E. Brinson and W. Dunstan has been obtained.

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1. Introduction

It is now an established fact that in doped semiconductors at low temperatures, electron–phonon interaction plays an important role for the phonon conductivity [1–4]. By considering the technological demands of silicon, very recently, one of the present authors [5] has explained phonon conductivity in intermediately Li-doped silicon. In the present paper, we have investigated the electron–phonon interaction and phonon conductivity in heavily doped silicon with $N_{\mathrm{ex}} > N_{\mathrm{c}}$, where N_{ex} is the donor concentration and N_{c} is the critical concentration of the donor at which the sample becomes metal introduced by Mott [6].

Experimentally, phonon conductivity in heavily doped n-type silicon has been investigated by Brinson and Dunstan [7]. In Sect. 2, we present the expression for the modified electron–phonon relaxation rate for heavily doped n-type silicon deduced recently [5] by introducing spherical-polar coordinates for the phonon polarization vectors in the general expression of Sota and Suzuki [8]. Section 3 presents the results of the calculation for the phonon conduction in As- and P-heavily doped silicon and their thorough analysis.

2. Theory

In impure semiconductors, when the concentration of donors or acceptors is low, the wave functions associated with them are localized, the electrons or holes are bound to the impurities and the system is regarded as non-metal. As the concentration of impurity atoms increases, the wave functions begin to overlap, the carriers become free and sample behaves like a metal. Such a transition from non-metallic to metallic state takes place in heavily doped semiconductors for carrier concentrations N_{ex} such that $N_{\mathrm{ex}} > N_{\mathrm{c}}$ (Mott [6]), where

$$N_{\mathrm{c}} = \left(\frac{0.25}{a^*}\right)^3 \tag{1}$$

where $a^* = \left(a^2 b\right)^{1/3}$ is the effective Bohr radius, and a and b are the transverse and longitudinal Bohr radii, respectively.

It is well known that thermal phonons are strongly scattered by free carriers in heavily-doped semiconductors. For instance, at low temperature in n-type Ge and GeSb, a large thermal resistance arises from the phonon scattering by free electrons. Phonon conductivity in heavily-doped n-type Ge has been analysed by many researchers [9,10] using the Ziman expression [11] for the electron–phonon relaxation rate. Ziman expression was derived for a single-valley potential and the effect of screening was not taken into account in the electron–phonon scattering processes.

Sota and Suzuki [8] investigated the electron–phonon interaction in heavily doped many-valley semiconductors. When a phonon propagates in the crystal, it disturbs the electron system through the electron–phonon interaction. The amount of perturbation varies from valley to valley depending on the strength of the electron–phonon coupling. At a particular temperature the electron population in a valley will be at its thermal equilibrium value. Due to the electron–phonon interaction, the electron population of a valley will deviate from the thermal equilibrium value. At low temperatures, the average gain or loss of energy by the electron is given by the average energy of a phonon at that temperature which is of the order of $k_{\mathrm{B}}T$. Due to the propagation of phonons, electron population in each valley will be changed and the phonons loose their energy through this process. For a metallic state, we have to take into account the screening effect by the conduction electrons. Sota and Suzuki obtained the general expression for the relaxation rate for a free electron by solving the equation of motion for the single particle density matrix within the self-consistent field approximation as

$$\frac{1}{\tau_{\mathrm{e-ph}}} = -\frac{q}{\rho v_\lambda} \mathrm{Im}\left\{ n R_{\mathrm{D}} E_{\mathrm{D}}^2 \left(\hat{e}_\lambda \cdot \hat{q}\right)^2 + R_{\mathrm{S}} E_{\mathrm{u}}^2 \sum_j U_{j\lambda}^2 \right\}. \tag{2}$$

Explicit expressions for $R_{\rm D}$ and $R_{\rm S}$ are given in Ref. [8] (Eqs. (48) and (49)). Here $E_{\rm D} = E_{\rm d} + E_{\rm u}/3$, where $E_{\rm d}$ and $E_{\rm u}$ are the dilatation and shear deformation potential constants, respectively. n is the number of conduction band minima; for silicon it is 6. In Eq. (2), $U_{j\lambda} = \hat{e}_\lambda \cdot \big(U^{(j)} - \mathbf{1}\big) \cdot \hat{q}$. The matrices $U^{(j)}$ for different values of the conduction band minima j can be obtained from the dyad $\big(\hat{k}(j) : \hat{k}(j)\big)$, where $\hat{k}(j)$ are the unit vectors pointing towards the bottom of the $j^{\rm th}$ valley of the conduction band minima. The unit vectors $\hat{k}(j)$ for six valleys of silicon are $(1,0,0)$, $(-1,0,0)$, $(0,1,0)$, $(0,-1,0)$, $(0,0,1)$ and $(0,0,-1)$. The $\hat{e}_\lambda(q)$, $\lambda = 1$, 2 and 3, are three phonon polarization vectors, with $\hat{e}_1(q)$ pointing along the propagation of the phonon wave vector $\boldsymbol{q}$. Assuming

$$\begin{aligned}
\hat{e}_1 &= \hat{\imath}\sin\theta\cos\phi + \hat{\jmath}\sin\theta\sin\phi + \hat{k}\cos\theta, \\
\hat{e}_2 &= \hat{\imath}\cos\theta\cos\phi + \hat{\jmath}\cos\theta\sin\phi - \hat{k}\cos\theta, \\
\hat{e}_3 &= -\hat{\imath}\sin\phi + \hat{\jmath}\cos\phi \qquad (3)
\end{aligned}$$

for the three phonon polarization vectors, and introducing the spherical polar coordinates in Eq. (2), the angular average for $\sum_j U_{j\lambda}^2$ over the solid angle dΩ for silicon are [5]

$$\Big\langle \sum_j U_{j1}^2 \Big\rangle = \frac{8}{15}\,, \qquad \Big\langle \sum_j U_{j2}^2 \Big\rangle = \frac{7}{15}\,, \qquad \Big\langle \sum_j U_{j3}^2 \Big\rangle = \frac{1}{3}\,.$$

3. *Results and discussion*

Phonon conductivity K for heavily doped n-type silicon has been calculated using the Callaway model [12] modified by Holland [13]. It is given by

$$\begin{aligned}
K &= CT^3\Bigg(\frac{1}{2v_{\rm l}}\int\limits_0^{\Theta_{\rm l}/T} \tau_{\rm l}(x)J_4(x){\rm d}x + \frac{1}{v_{\rm t}}\int\limits_0^{\Theta_{\rm t}'/T} \tau_{\rm t}(x)J_4(x){\rm d}x \\
&\quad + \frac{1}{v_{\rm t}}\int\limits_{\Theta_{\rm t}'/T}^{\Theta_{\rm t}/T} \tau_{\rm t}'(x)J_4(x){\rm d}x\Bigg), \qquad (4)
\end{aligned}$$

with

$$C = \frac{k_{\rm B}^4}{3\pi^2\hbar^3} \quad \text{and} \quad J_4(x) = \frac{x^4{\rm e}^x}{\big({\rm e}^x - 1\big)^2}.$$

$\Theta_{\rm l}$ and $\Theta_{\rm t}$ are calculated at the first-zone boundary frequencies of the phonon dispersion curve for the LA and TA branches, respectively, while $\Theta_{\rm t}'$ corresponds to the phonon frequency at $q_{\rm max}/2$ in TA branch. The $\tau_{\rm l}$, $\tau_{\rm t}$ and $\tau_{\rm t}'$ are the total relaxation times for the longitudinal, transverse first zone ($0 < q < q_{\rm max}/2$) and transverse second zone ($q_{\rm max}/2 < q < q_{\rm max}$), respectively. $x = \hbar\omega_{q\lambda}/(k_{\rm B}T)$, v_λ is the phonon velocity and $\omega_{q\lambda}$ is the phonon angular frequency. The total relaxation rate $\tau^{-1}(x)$ is

$$\tau^{-1}(x) \quad = \quad \tau_{\rm b}^{-1} + \tau_{\rm pt}^{-1} + \tau_{\rm 3ph}^{-1} + \tau_{\rm e-ph}^{-1}, \tag{5}$$

where $\tau_{\rm b}^{-1} = v_\lambda/L_{\rm C}$ is the phonon relaxation rate due to the boundary scattering. $L_{\rm C}$ is the Casimir length. $\tau_{\rm pt}^{-1} = A\omega_{q\lambda}^4$ represents relaxation rate due to point defects. $\tau_{\rm 3ph}^{-1}$ is the relaxation rate which arises from the phonon-phonon interactions. It is equal to $B_{\rm l}\omega_{q\lambda}^2 T^3$ for longitudinal phonons. For the transverse branch, $\tau_{\rm 3ph}^{-1}$ is equal to $\tau_{\rm nt}^{-1} + \tau_{\rm ut}^{-1}$. $\tau_{\rm nt}^{-1}$ is equal to $B_{\rm nt}\omega_{q\lambda}T^4$. $\tau_{\rm ut}^{-1} = 0$ for $0 < q < q_{\rm max}/2$ and it is equal to $B'_{\rm ut}\omega_{q\lambda}^2/\sinh x$ in the region $q_{\rm max}/2 < q < q_{\rm max}$ of the dispersion curve. $\tau_{\rm e-ph}^{-1}$ is given by Eq. (2).

Using Eq. (4), phonon conductivity K of heavily-doped n-type silicon sample for $N_{\rm ex} > N_{\rm c}$ was calculated. The values of different parameters used in the calculations are given in Table 1. We have used the longitudinal phonon velocity $v_1 = 9.33 \times 10^5$ cm/s and transverse phonon velocity, $v_2 = v_3 = 5.42 \times 10^5$ cm/s, $m^* = 0.33\, m_{\rm el}$, $\rho = 2.33$ g/cm^{-3} and $\epsilon_0 = 11.4$.

TABLE 1. Values of the different parameters used in the present calculations to calculate phonon conductivity for the samples S I-17 and S I-19.

Sample	S I-17	S I-19
$N_{\rm ex}$ - donor electron concentration	4.45 $\times 10^{18}$	5.67 $\times 10^{19}$
$E_{\rm u}$ - shear deformation potential	4 eV	5 eV
$E_{\rm d}$ - dilation deformation potential	3 eV	2 eV
$L_{\rm C}$ - Casimir length	0.06544 cm	0.22544 cm
A - point defect parameter	4.17 $\times 10^{-44}$ s^3	9.87 $\times 10^{-44}$ s^3
$B_{\rm l}$ - longitudinal phonon-phonon scattering parameter	1.34 $\times 10^{-22}$ sK^{-3}	5.73 $\times 10^{-24}$ sK^{-3}
$B_{\rm nt}$ - transverse phonon-phonon scattering parameter (N-process)	9.31 $\times 10^{-14}$ K^{-4}	1.90 $\times 10^{-12}$ K^{-4}
$B_{\rm ut}$ - transverse phonon-phonon scattering parameter (U-process)	4.37 $\times 10^{-17}$ K^{-4}	3.79 $\times 10^{-17}$ K^{-4}
τ'	6.0 $\times 10^{-12}$ s	4.5 $\times 10^{-12}$ s
ν'	5.2 $\times 10^{14}$ s^{-1}	5.0 $\times 10^{14}$ s^{-1}

In Fig. 1, we show the relaxation rates $\tau_{\mathrm{e-ph}}^{-1}$, τ_{b}^{-1}, τ_{pt}^{-1} and τ_{3ph}^{-1} of the incoming longitudinal phonons as functions of the phonon angular frequency ω at $T = 15$ K. From Fig. 1 it is observed that τ_{pt}^{-1} plays an important role in the frequency range $2 \times 10^{12} < \omega < 2 \times 10^{13}$ Hz. $\tau_{\mathrm{e-ph}}^{-1}$ is also important in the frequency range $1 \times 10^{12} < \omega < 1.5 \times 10^{13}$ Hz. At $T = 15$ K, the three-phonon interaction is less significant. τ_{b}^{-1} is important at low frequency and less important at the high frequency side.

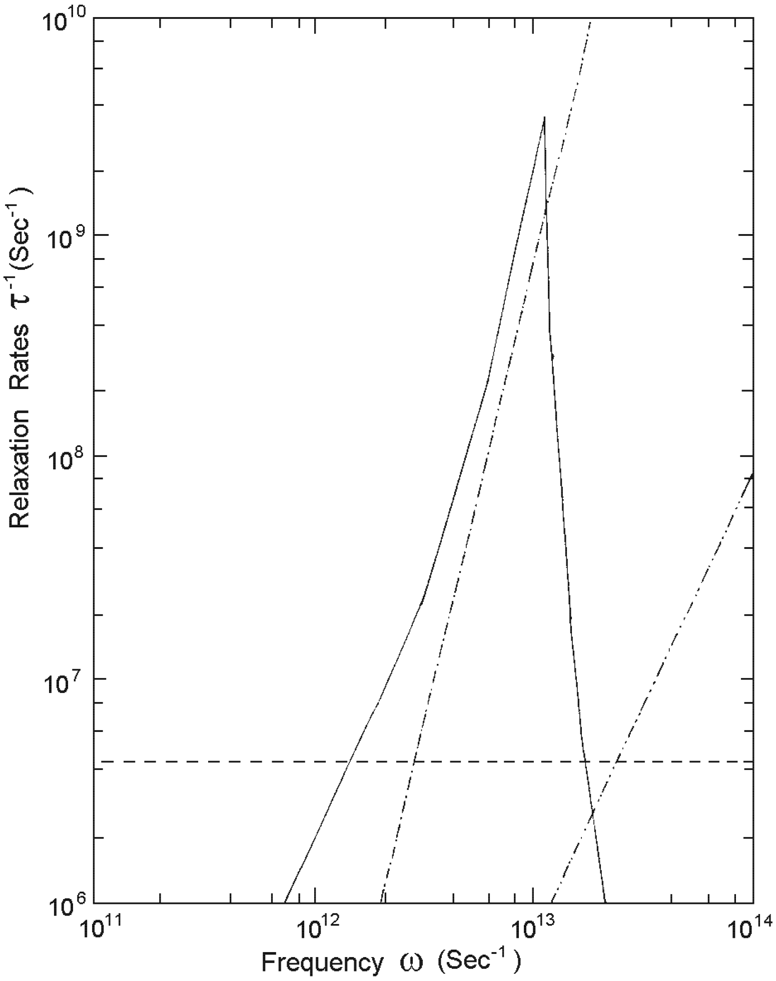

Fig. 1. Relaxation rates τ^{-1} of the incoming longitudinal phonons as a funtion of angular frequency ω in As-doped *silicon (sample SI-19 of Ref. [7]) with $E_{\mathrm{u}} =$ 5 eV, $E_{\mathrm{d}} = 2$ eV at $T = 15$ K. Solid, dashed, dot-dashed and dot-dot-dashed lines represent, respectively, electron-phonon scattering, boundary scattering, point defect scattering and phonon–phonon scattering.*

The phonon conductivity K for the samples S I-17 and S I-19 of Brinson and Dunstan [7] has been calculated using Eq. (4). It is presented in Figs. 2 and 3 together with the experimental results. A good agreement between the theoretical and experimental results [7] has been obtained, except for the lowest available experimental points. When the best fit was made for the low temperatures, then it becomes impossible to get a reasonable fit for the higher temperatures.

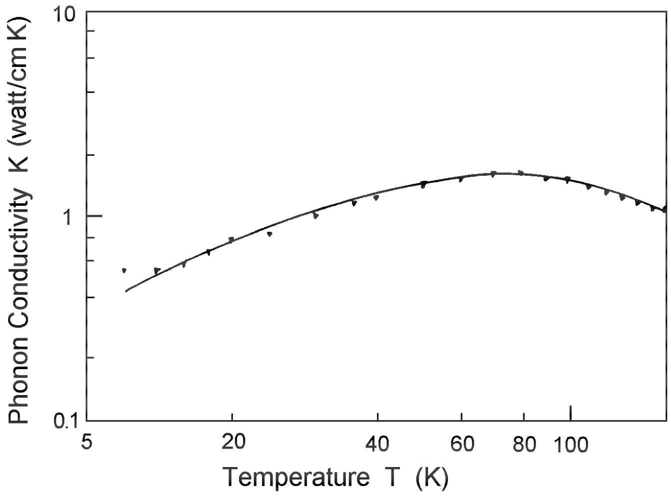

Fig. 2. Phonon conductivity obtained by the present calculation and the experimental points for the sample S I-19 of Ref. [7]. Values of the different parameters are given in Table 1.

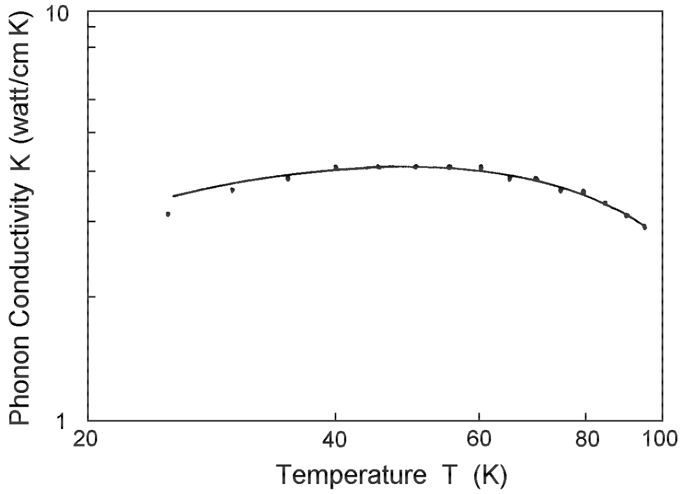

Fig. 3. Phonon conductivity obtained by the present calculation and the experimental points for the sample S I-17 of Ref. [7]. Values of the different parameters are given in Table 1.

For the sample S I-17, P-doped silicon, $N_{\mathrm{ex}} = 4.45 \times 10^{18}$ cm^{-3} and $N_{\mathrm{c}} = 3.45 \times 10^{18}$ cm^{-3}, and for the sample S I-19, As-doped silicon, $N_{\mathrm{ex}} = 5.67 \times 10^{19}$ cm^{-3} and $N_{\mathrm{c}} = 4.46 \times 10^{18}$ cm^{-3}. For phonon conductivity calculation, we have chosen higher values for the point-defect scattering parameter A than reported earlier [14]. The larger value of A is justified in the present case because of higher donor concentration [15,16]. L_{C}, the Casimir length, was adjusted to the experimental result at the lowest available temperature because the boundary scattering is most effective at low temperature. ν' is a parameter that depends on the intervalley scattering rate of the electron due to impurities and τ' is a parameter that represents the total relaxation time of the electron. Adjusted values of the parameters τ' and ν' are close to the values reported earlier for Ge [8,16]. Values of shear deformation potential E_{u} are smaller than the value reported for lightly doped n-type silicon [14], which is justified because of the higher donor concentration. For Ge it has been observed that E_{d} is always negative [14,16], but for the present case we had to take a positive value of E_{d} in order to get the best fit to the experimental results. For the lightly doped Li-O silicon, E_{d} was also taken positive to get the best fit to the phonon conductivity curve [2]. Moreover, it has been found by Cheung and Barrie [17] that for n-type silicon, a positive value of E_{d} is necessary in order to explain the shift of the donor energy levels with temperature and the value of E_{d} chosen here is close to the value reported experimentally [17].

4. *Conclusion*

Calculated values of phonon conductivity for samples S I-17 and S I-19 together with the experimental results of Brinson and Dunstan [7] show that the theory Sota and Suzuki [8] for the electron-phonon relaxation rate in heavily-doped n-type silicon can explain the data fairly well, except for the lowest available temperature. The discrepancies may be due to the inaccuracy in the measurement of the phonon conductivity at the lowest temperatures.

A better fit to the experimental points at all temperatures for the present samples requires reliable experimental phonon dispersion curves for heavily-doped n-type silicon samples [18], but these data are not available at present. We also feel that more experimental work on phonon conductivity K for heavily doped n-type silicon is necessary over a broader temperature range.

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FONONSKA VODLJIVOST U JAKO PUNJENOM SILICIJU N-TIPA

Ako je koncentracija donora u poluvodiču n-tipa $N_{\rm ex} > N_{\rm c}$, gdje je $N_{\rm c}$ kritična koncentracija koju je definirao Mott, uzorak postaje metal. Izraz za brzinu elektronsko-fononskog smiraja u takvim poluvodičima izveli su T. Sota i K. Suzuki samosuglasnom metodom. U nedavnom radu ga je izmijenio M. K. Roy i ovdje se primjenjuje kako bi se uzela u obzir stvarna slika raspršenja fonona u jako punjenom siliciju n-tipa. Primjenjuje se kutni prosjek potencijala deformacije za različite polarizacijske vektore λ koji su izvedeni uvođenjem sfernih koordinata. Izračunali smo fononsku vodljivost K za silicij punjen s As i P za $N_{\rm ex} > N_{\rm c}$. Postigli smo dobro slaganje naših izračunatih vrijednosti s mjernim podacima M. E. Brinsona i W. Dunstana.