Eur. Phys. J. B **30**, 289–293 (2002)
DOI: 10.1140/epjb/e2002-00381-8

THE EUROPEAN PHYSICAL JOURNAL B

Electron-phonon interaction and phonon conductivity in Li-doped silicon with intermediate donor concentration

M.K. Roy[a]

Department of Physics, University of Chittagong, Chittagong, Bangladesh

Received 18 May 2001 / Received in final form 4 July 2002
Published online 19 December 2002 – © EDP Sciences, Società Italiana di Fisica, Springer-Verlag 2002

Abstract. Phonon conductivity in intermediately doped n-type silicon still remains unexplained. In this paper we have calculated the phonon conductivity in Li-doped silicon for $N_{ex} < N_c$ using Mikoshiba's inhomogeneity model. We have introduced spherical polar coordinates for the phonon polarization vectors in Sota and Suzuki's theory in order to take into account the realistic picture of the scattered phonons. Deformation potential for different polarizations λ has been evaluated for the metallic region. Present calculations show that Mikoshiba's inhomogeneity model is able to explain the phonon conductivity of Li-doped silicon having intermediate donor concentration very well.

PACS. 63.20.kr Phonon-electron and phonon-phonon interactions – 66.70.+f Nonelectronic thermal conduction and heat-pulse propagation in solids; thermal waves

1 Introduction

Very recently, the present author (with the co-author) [1,2] has explained phonon conductivity in intermediately doped n-type germanium. By considering the technological demands of silicon, in the present paper, we have investigated the electron-phonon interaction and phonon conductivity in Li-doped silicon having $N_{ex} < N_c$, where N_{ex} is the donor concentration and N_c is the critical concentration of the donor at which the sample becomes metal. Experimentally phonon conductivity for such intermediately doped n-type silicon has been investigated by many researchers [3–5]. In order to explain phonon conductivity for such type of semiconductors, we have used the inhomogeneity model of Mikoshiba [6] in which the impurity states are regarded as the spatial mixture of metallic and non-metallic regions.

In Section 2 we have presented the detail procedure for the calculation of electron-phonon relaxation rate expression in heavily doped n-type silicon. Section 3 provides the results of the calculations for the phonon conductivity in Li-doped silicon having intermediate donor concentration and presents a thorough analysis of the obtained results.

2 Theory

Following Mikoshiba's inhomogeneity model [6], for intermediately doped semiconductors in which $N_{ex} < N_c$, we can spatially separate the charge centers into metallic and non-metallic regions, where

$$N_c = (0.25/a^*)^3 \tag{1}$$

with $a^* = (\mathrm{a}^2\mathrm{b})^{1/3}$ is the effective Bohr radius [7] and 'a' and 'b' are the transverse and longitudinal Bohr radii respectively. In the non-metallic region the charged centers are localized and screening effect can be ignored safely in order to investigate electron-phonon interaction. On the other hand, in the metallic region the wave function of the donor atoms overlaps with one another and electrons become free. Here, the electron-phonon interaction is strongly affected by the screening effect of the conduction electrons.

In the aforesaid model, in non-metallic region there is no neighbor closer than the radius $r_c = (144/\pi^2)^{1/3}a^*$. Hence, the concentration of non-metallic donor centers are:

$$N_{nm} = N_{ex}\,\exp(-t_c) \tag{2}$$

with

$$t_c = \frac{4\pi}{3}N_{ex}r_c^3$$

and the concentration of metallic states is given by

$$N_m = N_{ex}[1 - \exp(-t_c)]. \tag{3}$$

For the metallic region, the donor states merge with the conduction band. Sota and Suzuki [8] derived the

[a] e-mail: mkroy@ctgu.edu

general expression of electron-phonon relaxation rate in metallic region following self-consistent method as:

$$\tau_m^{-1} = -\left(\frac{q}{\rho v_\lambda}\right) \mathrm{Im}\left[nR_D E_D^2 \left(\hat{e}_\lambda \cdot \hat{q}\right)^2 + R_S E_u^2 \left(\sum_j U_{j\lambda}^2\right)\right]. \quad (4)$$

Explicit expressions for R_D and R_S are given in reference [8] (Eq. (48) and Eq. (49) therein). Here $E_D = E_d + E_u/3$; E_d and E_u are the dilatation and shear deformation potential constant respectively. The 'n' is the number of conduction band minima and for silicon it is 6. The $\hat{e}_\lambda(q)$ are the three phonon polarization vectors with $\lambda = 1$, 2 and 3. Explicit expression for τ_m^{-1} depends on the choice of the phonon polarization vectors e_λ. In order to take into account the scattered phonons, here we have introduced the spherical polar coordinates for the phonon polarization vectors. We have pointed $\hat{e}_1$ along the propagation of the phonon wave vector $\mathbf{q}$ and chosen:

$$\hat{e}_1 = \hat{i}\sin\theta\,\cos\phi + \hat{j}\sin\theta\,\sin\phi + \hat{k}\cos\theta$$

$$\hat{e}_2 = \hat{i}\cos\theta\,\cos\phi + \hat{j}\cos\theta\,\sin\phi - \hat{k}\sin\theta$$

$$\hat{e}_3 = -\hat{i}\sin\phi + \hat{j}\cos\phi \quad (5)$$

for the three phonon polarization vectors. In equation (4),

$$U_{j\lambda} = \hat{e}_\lambda \cdot \left(U^{(j)} - \mathbf{1}\right) \cdot \hat{q}. \quad (6)$$

The values of the matrices $U^{(j)}$ for the different values of the conduction band minima 'j' can be obtained from the dyad $(\hat{k}^{(j)} : \hat{k}^{(j)})$, where $\hat{k}^{(j)}$ are the unit vectors pointing towards the bottom of the jth valley of the conduction band. $U_{j\lambda}$ for different values of the conduction band minima 'j' and polarizations 'λ' can be evaluated from equation (6).

Here, we have obtained the angular average for $\sum_j U_{j\lambda}^2$ over the solid angle $\mathrm{d}\Omega$ for silicon for different value of λ as:

$$\left\langle \sum_j U_{j\lambda}^2 \right\rangle = \frac{8}{15} \text{ for } \lambda = 1, \quad \left\langle \sum_j U_{j\lambda}^2 \right\rangle = \frac{7}{15} \text{ for } \lambda = 2$$

and

$$\left\langle \sum_j U_{j\lambda}^2 \right\rangle = \frac{1}{3} \text{ for } \lambda = 3.$$

For non-metallic donor states we have used the electron-phonon relaxation rate expression derived by Roy and Sood [9] for elastic τ_{el}^{-1}, inelastic τ_{inel}^{-1} and thermally assisted phonon absorption prosses τ_{abs}^{-1}. To derive those expressions anisotropic donor electron wave function has been used in the deformation potential theory. Here we present only the expression for elastic process,

$$\tau_{el}^{-1} = \frac{\omega_{q\lambda}^4}{4\pi\rho^2 v_\lambda^2} \sum_{\lambda'} \frac{1}{v_{\lambda'}^5} \frac{4\,(4\Delta)^2}{[(\hbar\omega_{q\lambda})^2 - (4\Delta)^2]^2 + 4\Gamma^2(4\Delta)^2} \times \left[[N_s(T) + N_f(T)] \sum_{m=1}^{5} \left[\langle (M_{0m}^{q'\lambda'})^2\rangle \langle (M_{m0}^{q\lambda})^2\rangle\right] + N_f(T) \left[\frac{(\hbar\omega_{q\lambda})^2 + (4\Delta)^2}{2(\hbar\omega_{q\lambda})^2}\right] \sum_{n=1}^{5} \left[\langle (M_{0n}^{q'\lambda'})^2\rangle \times \sum_{m=1}^{5} \langle (M_{m0}^{q\lambda})^2\rangle\right]\right]. \quad (7)$$

In equation (7), $N_s(T)$ and $N_f(T)$ are the density of electron in the singlet, $1s(A_1)$ and fivefold degenerate, $1s(E+T_2)$ states respectively corresponding to nonmetallic region. $M_{mn}^{q\lambda}$ represents the matrix element for the scattering of phonon having wave vector $\mathbf{q}$ and polarization λ by the bound donor electron from a state 'm' to a state 'n'. The '4Δ' is the chemical shift between $1s(A_1)$ and $1s(E+T_2)$ states and Γ is the total level width. Explicit expression for $M_{mn}^{q\lambda}$, τ_{inel}^{-1}, τ_{abs}^{-1} and Γ can be found in reference [9]. The relaxation rates for phonon due to different scattering process in the non-metallic states is:

$$\tau_{nm}^{-1} = \tau_{el}^{-1} + \tau_{inel}^{-1} + \tau_{abs}^{-1}. \quad (8)$$

3 Result and discussion

For the calculation of phonon conductivity 'K' we have used the Callaway model [10] modified by Holland [11] which is given by:

$$K = K_l + K_{t_1} + K_{t_2} \quad (9)$$

where

$$K_l = \frac{k_B^4 T^3}{6\pi^2\hbar^3 v_l} \int_0^{\Theta_l/T} \tau_{cl}(x) J_4(x) \mathrm{d}x \quad (10)$$

$$K_{t1} = \frac{k_B^4 T^3}{3\pi^2\hbar^3 v_t} \int_0^{\Theta_t'/T} \tau_{ct}(x) J_4(x) \mathrm{d}x \quad (11)$$

$$K_{t2} = \frac{k_B^4 T^3}{3\pi^2\hbar^3 v_t} \int_{\Theta_t'/T}^{\Theta_t/T} \tau_{ct}'(x) J_4(x) \mathrm{d}x \quad (12)$$

with $J_4(x) = \frac{x^4 \mathrm{e}^x}{(\mathrm{e}^x - 1)^2}$.

The Θ_l and Θ_t are calculated at the first zone boundary frequencies of the phonon dispersion curve for the LA and TA branches respectively while Θ_t' corresponds to the phonon frequency at $q_{max}/2$ in TA branch. The τ_{cl}, τ_{ct} and τ_{ct}' are the total relaxation time for the longitudinal,transverse first zone ($0 < q < q_{max}/2$) and transverse

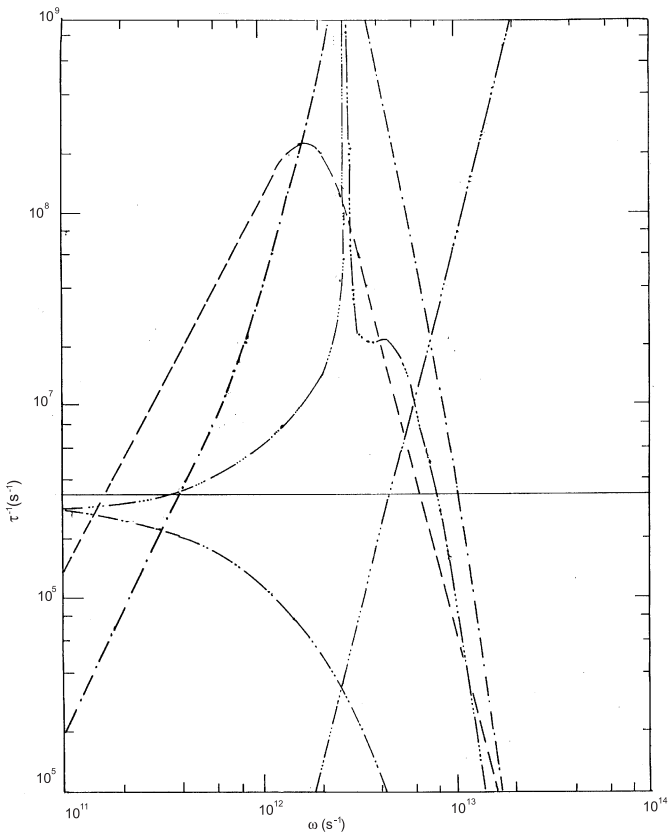

Fig. 1. Relaxation rates τ^{-1} of the incoming longitudinal phonons as a function of angular frequency ω in Li-doped silicon (sample-9 of Ref. [5]) with $E_u = 13$ eV, $E_d = 4$ eV at $T = 5$ K. Solid line is for boundary scattering, - - - - represents metallic part, — · — · — represents elastic scattering, — · · — · · — represents inelastic scattering, — · · · — · · · — represents point defect scattering and — · · · · — · · · · — is for thermally assisted phonon absorption process.

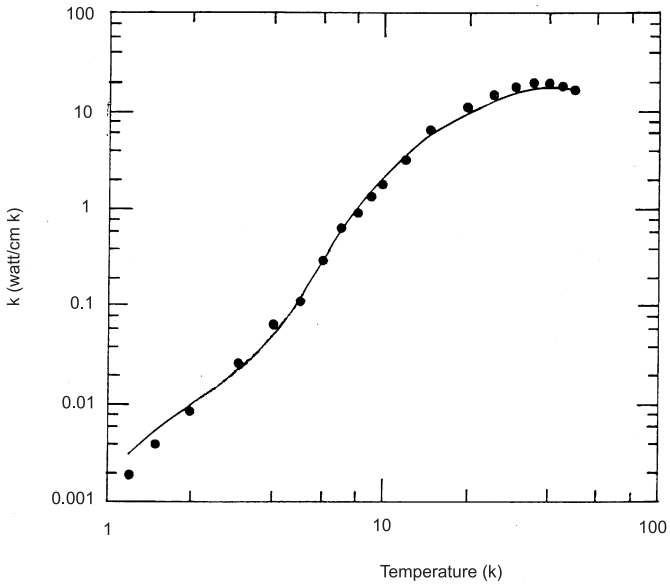

Fig. 2. Phonon conductivity obtained by the present calculations and the experimental points for Li-doped silicon (sample-8 of Ref. [5]). Values of the different parameters are given in Table 1.

second zone respectively. $x = \frac{\hbar\omega_{q\lambda}}{k_B T}$; v_λ is the phonon velocity; $\omega_{q\lambda}$ the phonon angular frequency. The total relaxation rate $\tau^{-1}(x)$ is

$$\tau^{-1}(x) = \tau_b^{-1} + \tau_{pt}^{-1} + \tau_{3ph}^{-1} + \tau_m^{-1} + \tau_{nm}^{-1} \qquad (13)$$

with $\tau_b^{-1} = \frac{v_\lambda}{L_c}$; L_c is the Casimir length, $\tau_{pt}^{-1} = A\omega_{q\lambda}^4$; $\tau_{3ph}^{-1} = B_l\omega_{q\lambda}^2 T^3$ for the longitudinal phonons. For the transverse branch τ_{3ph}^{-1} is equal to $B_t\omega_{q\lambda}T^4$ for $0 < q < q_{max}/2$ and it is equal to $B_t'\omega^2/\sinh x$ in the region $q_{max}/2 < q < q_{max}$ of the phonon dispersion curve. Expressions for τ_m^{-1} and τ_{nm}^{-1} are given by equations (4) and (8) respectively.

Figure 1 shows the relaxation rate τ_{el}^{-1}, τ_{inel}^{-1}, τ_{abs}^{-1}, τ_m^{-1}, τ_b^{-1}, τ_{pt}^{-1} *versus* angular frequency ω at $T = 5$ K for incoming longitudinal phonons for $N_{ex} = 5.2 \times 10^{17}/\text{cm}^3$. As three phonon processes are negligible at $T = 5$ K, so it has not been shown in Figure 1. From Figure 1 it is observed that τ_m^{-1} plays an important role in the frequency range $1 \times 10^{11} < \omega < 8.5 \times 10^{12}$ Hz. For non-metallic region τ_{el}^{-1} plays a very important role along with τ_{abs}^{-1} in the phonon conduction process whereas τ_{inel}^{-1} is less significant. So it is remarkable to mention here that at low temperature electron-phonon interaction plays the vital role in the phonon scattering process both for non-metallic and metallic regions. Using equation (9), the phonon conductivity 'K' of Li-doped silicon is calculated upto $T = 50$ K. Theoretical results obtained from our present calculations together with the experimental results of Fortier and Suzuki [5] for two samples with $N_{ex} < N_c$ are shown in Figures 2 and 3 respectively. Values of different parameters used in our present calculations for different samples are given in Table 1. For Li-doped silicon $4\Delta = 1.8$ meV [12]. In the present calculations, we have used $v_1 = 9.33\times10^5$ cm/s, $v_2 = v_3 = 5.42\times10^5$ cm/s, crystal density $\rho = 2.33$ gm/cm^3. With the experimental value of ionization energy for Li doped silicon, $E_o = 0.033$ eV for the $1s$ state the calculated value of $a = 24.65$ Å and $b = 11.24$ Å are used [13,14].

For lightly doped Li-doped silicon, value of the point defect parameter 'A' taken by Fortier and Suzuki [5] is 1.32×10^{-45} s^3. For the present samples we have chosen higher values of the point defect scattering parameter 'A' than that of the lightly doped samples. Increased value of 'A' is justified in the present case because of higher donor concentration [1,2,15]. In Figure 2 L_c was adjusted to get the best fit with the experimental phonon conductivity 'K'. For sample-8 the reported value of L_c is 0.265 cm [5]. But in Figure 3 for sample-9 of reference [5] we have taken the reported value of L_c to get the best fit. Adjusted value of the parameters τ' and ν' are not far away from the values reported for Ge by Roy and Deb [1,2] as well as by Sota and Suzuki (τ'=10^{-13} to

Table 1. Values of the different parameters used in the present calculations to calculate phonon conductivity in different Li-doped silicon.

Sample of Ref. [5]	Donor conentration N_{ex}/cm^3	Casimir length L_c in cm	Dilatation deformation potential E_d in eV	Shear deformation potential E_u in eV	Point defact parameter A in sec^3	Long. 3-phonon scattering parameter B_l in sec K^{-3}	Trans. 3-phonon scattering parameters		ι' in sec	ν' of sec^{-1}
							B_t in K^{-4}	B'_t in sec		
8	2.0×10^{17}	0.1254	3	12	4.45×10^{-45}	1.18×10^{-24}	$1.95 \times 10.^{-13}$	4.96×10^{-18}	9.00×10^{-13}	20×10^{11}
9	5.2×10^{17}	0.2600	4	13	6.83×10^{-45}	8.90×10^{-25}	2.71×10^{-14}	4.37×10^{-18}	3.25×10^{-13}	60×10^{11}

10^{-14} sec and $\nu' = 10^{11}$ to 10^{12} s^{-1}) [8]. In our present calculations we have observed that three-phonon processes are less important in intermediately doped samples for $T < 50$ K. For silicon reported value of B_l, B_t and B'_t are $B_l = 2.0 \times 10^{-24}$ $s\,deg^{-3}$, $B_t = 9.3 \times 10^{-13}$ deg^{-3}, $B'_t = 5.5 \times 10^{-18}$s [11]. As the three-phonon processes are related with the anharmonicity of crystal lattice, so for higher concentration of impurity atoms lower values of 3-phonon parameters are expected.

Figure 3 shows (for sample-9 of Ref. [5]) that our calculated values slightly overestimate the experimental result around $T = 10$ K to some extent. Here we have adjusted E_d and E_u at $T = 5$ K. Watkins and Ham's electron paramagnetic resonance experiment on Lithium doped silicon shows that $E_u = 11.4 \pm 1.1$ eV [16]. Values of the shear deformation potential E_u that we chosen in the present calculation are nearly same as in the calculations of phonon conductivity for n-type silicon by Fortier and Suzuki ($E_u = 11.4$ eV) [5] and Watkins and Hamé [16]. For germanium it has been observed that E_d is always negative [1,2,5,17,18], but for silicon we have to take positive values of E_d in order to get the best fit with the experimental result. For lightly Li-O doped silicon samples we had to take positive value of E_d (= 5 eV) to get the best fit with the experimental phonon conductivity curve [9]. Moreover, it has been found by Cheung and Barrie [19] that for n-type silicon positive value of E_d (= 10 eV) is necessary to explain the shift of the donor energy levels with temperature. It is important to mention here that Myszkowski and Rogola [20] pointed out that the dilatation deformation potential E_d for silicon is positive though it is negative for germanium. The value of E_d predicted by them is 2.6 eV.

From our present calculations of phonon conductivity 'K' for intermediately Li-doped silicon, it is observed that Mikoshiba model is successful to explain fairly well the experimental results except at very low temperatures $T < 2$ K. At very low temperature other scattering process like hopping between unoccupied and occupied donor centers may play an important role [21] which need further investigation. The use of such inhomogeneity model to explain phonon conductivity in intermediately doped samples receives support on the ground that in n-type

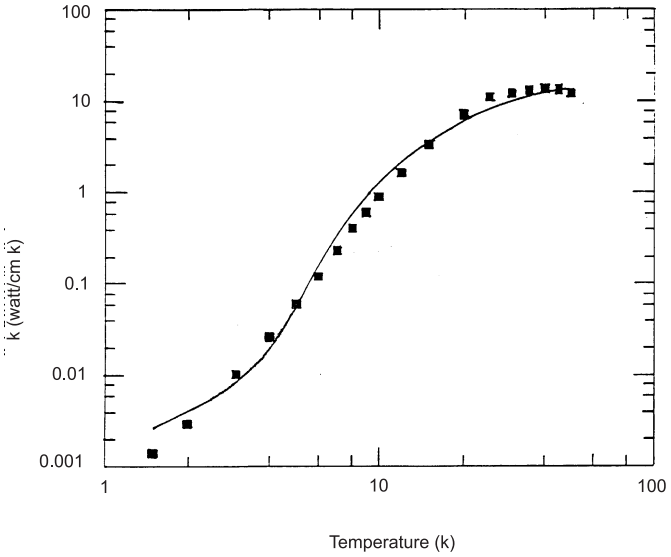

Fig. 3. Phonon conductivity obtained by the present calculations and the experimental points for Li-doped silicon (sample-9 of Ref. [5]). Values of the different parameters are given in Table 1.

semiconductor binding energy of the donor electron decreases gradually with the increase of donor concentration and the sample becomes metal at a critical donor concentration N_c. This decrease of donor ionization energy with concentration is a phase transition of second order. Such type of model has already been used by Szczybowski and Czapla [22] to calculate electron concentration in InAs film and found good agreement with the experimentally obtained result.

Detail adjustments with the experimental point at high temperature for the present samples require experimental phonon dispersion curve for intermediately doped samples [23] that are not available at present and it will also be interesting to investigate the effect of hopping at very low temperature for such type of semiconductors.

References

1. M.K. Roy, B. Deb, Sol. State Phenomena **55**, 164 (1997)
2. M.K. Roy, B.K. Deb, Phys. Rev. B **57**, 12229 (1998)
3. L.J. Challis, A.P. Heraud, V.W. Rampton, M.K. Saker, M.N. Wybourne, *Phonon Scattering in Condensed Matter: Procedings of the Fourth International Conference, University of Stuttgart, Fed. Rep. of Germany, August 22-26, 1983, pp. 358–360*
4. D. Fortier, K. Suzuki, J. Phys. France **37**, 143 (1976)
5. D. Fortier, K. Suzuki, Phys. Rev. B **9**, 2530 (1974)
6. N. Mikoshiba, Rev. Mod. Phys. **40**, 833 (1968)
7. N.F. Mott, Can., J. Phys. **34**, 1356 (1956)
8. T. Sota, K. Suzuki, J. Phys. C **15**, 6991 (1982)
9. M.K. Roy, K.C. Sood, Phys. Rev. B **47**, 3126 (1993)
10. J. Callaway, Phys. Rev. **113**, 1046 (1959)
11. M.G. Holland, Phys. Rev. **132**, 2461 (1963)
12. R.L. Aggarwal, P. Fisher, V. Mourzine, A.K. Ramdas, Phys. Rev. **138**, A882 (1965)
13. F. Bassani, G. Ladonisi, B. Preziosi, Rep. Prog. Phys. **37** 1101 (1974)
14. K.F. Berggren, Phil. Mag. **27**, 1027 (1973)
15. R. Berman, J.C.F. Brock, Proc. R. Soc. London, A **289**, 46 (1965)
16. G.D. Watkins, F.S. Ham, Phys. Rev. B **1**, 4071 (1971)
17. M.K. Roy, K.C. Sood, Phys. Rev. B **44**, 11085 (1991)
18. K.C. Sood, M.K. Roy, Phys. Rev. B **46**, 7486 (1992)
19. C.Y. Cheung, R. Barrie, Can. J. Phys. **45**, 1421 (1967)
20. A. Myszkowski, M. Rogala, Phys. Rev. **168** 768 (1968)
21. Z.W. Gortel, J. Phys. C **9**, 693 (1976)
22. J. Szczybowski, A. Czapla, Thin Solid Films **46**, 127 (1977)
23. K.C. Sood, M.K. Roy, J. Phys. Cond. Matt. **5**, 301 (1993)