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

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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 \( \lambda \) 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 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:

\[
N_{nm} = N_{ex} \exp(-t_c) \quad (2)
\]

with \( t_c = 4\pi^2/3N_{ex}r_c^3 \) and the concentration of metallic states is given by

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

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

\[
N_c = (0.25/a^*)^3 \quad (1)
\]

with \( a^* = (a^2b)^{1/3} \) 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.

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\]

For the metallic region, the donor states merge with the conduction band. Sota and Suzuki [8] derived the...
The values of the matrices $U$ for the three phonon polarization vectors. In equation (4),

$$
\tau_{m}^{-1} = \left(\frac{q}{\rho \nu_{\lambda}}\right) \text{Im} \left[ n R_{D} E_{D}^{2} (\hat{e}_{\lambda} \cdot \hat{q})^{2} + R_{S} E_{u}^{2} \left( \sum_{j} U_{j,\lambda}^{2} \right) \right].
$$

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 $\tau_{m}^{-1}$ depends on the choice of the phonon polarization vectors $\hat{e}_{\lambda}$. 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 $\hat{e}_{i}$ along the propagation of the phonon wave vector $\mathbf{q}$ and chosen:

$$
\hat{e}_{1} = \hat{i} \sin \theta \cos \phi + \hat{j} \sin \theta \sin \phi + \hat{k} \cos \theta
$$

$$
\hat{e}_{2} = \hat{i} \cos \theta \cos \phi + \hat{j} \cos \theta \sin \phi - \hat{k} \sin \theta
$$

$$
\hat{e}_{3} = -\hat{i} \sin \phi + \hat{j} \cos \phi
$$

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

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

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 '\lambda' can be evaluated from equation (6).

Here, we have obtained the angular average for $\sum_{j} U_{j,\lambda}^{2}$ over the solid angle $d\Omega$ for silicon for different value of $\lambda$ 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 $\tau_{el}^{-1}$, inelastic $\tau_{inel}^{-1}$ and thermally assisted phonon absorption process $\tau_{abs}^{-1}$. 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,

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

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. $M_{q,\lambda}^{n}$ represents the matrix element for the scattering of phonon having wave vector $\mathbf{q}$ and polarization $\lambda$ by the bound donor electron from a state 'n' to a state 'n'. The '4\Delta' is the chemical shift between $1s(A_{1})$ and $1s(E + T_{2})$ states and $\Gamma$ is the total level width. Explicit expression for $M_{q,\lambda}^{n}, \tau_{inel}^{-1}, \tau_{abs}^{-1}$ and $\Gamma$ can be found in reference [9]. The relaxation rates for phonon due to different scattering process in the non-metallic states is:

$$
\tau_{nm}^{-1} = \tau_{el}^{-1} + \tau_{inel}^{-1} + \tau_{abs}^{-1}.
$$

### 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:

$$
K = K_{1} + K_{11} + K_{12}
$$

where

$$
K_{1} = \frac{k_{B} \tau_{3}^{3}}{6 \pi^{2} \hbar^{3} v_{t}} \int_{0}^{\Theta_{f}/T} \tau_{d}(x) J_{4}(x) dx
$$

$$
K_{11} = \frac{k_{B} \tau_{3}^{3}}{3 \pi^{2} \hbar^{3} v_{t}} \int_{0}^{\Theta_{f}/T} \tau_{ct}(x) J_{4}(x) dx
$$

$$
K_{12} = \frac{k_{B} \tau_{3}^{3}}{3 \pi^{2} \hbar^{3} v_{t}} \int_{0}^{\Theta_{f}/T} \tau_{ct}(x) J_{4}(x) dx
$$

with $J_{4}(x) = \frac{x^{3}}{e^{x} - 1}$.

The $\Theta_{f}$ and $\Theta_{t}$ are calculated at the first zone boundary frequencies of the phonon dispersion curve for the LA and TA branches respectively while $\Theta_{f}$ corresponds to the phonon frequency at $q_{max}/2$ in TA branch. The $\tau_{ct}$, $\tau_{del}$ and $\tau_{ct}'$ are the total relaxation time for the longitudinal, transverse first zone $(0 < q < q_{max}/2)$ and transverse...