Low-temperature magneto-phonon conductivity of lightly doped Si

Surendra Singh and G. S. Verma
Physics Department, Banaras Hindu University, Varanasi-221005, India
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The relative importance of the elastic and inelastic phonon scattering by shallow acceptors to the low-temperature magneto-thermal conductivity of boron-doped Si is studied in the present paper. It is shown that in the temperature range 1–5 K and for magnetic fields up to 55 kG the elastic scattering makes the major contribution towards phonon resistivity. The magnetic field removes the degeneracy of the ground state and the phonon conductivity first falls as the level splittings become comparable to the dominant phonon energies ($\sim 4k_BT$) and then rises rapidly when the splittings become $\gg k_BT$. These features are reflected in our calculations. The discrepancy between theory and experiment regarding the absolute values of the ratio $[\kappa(H)/\kappa(H=0)]$ still remains unresolved with the present magnetic-level structure and g values.

I. INTRODUCTION

The effects of the magnetic field on the phonon conductivity of p-type Ge and Si have been studied by Challis and Halbo.[1] They explained their experimental results on the basis that the magnetic field removes the degeneracy of the ground state and the phonon conductivity first falls as the level splittings become comparable to the dominant phonon energies ($\sim 4k_BT$) and then rises rapidly when the splittings become $\gg k_BT$. However, they did not give any quantitative explanation of their experimental observations. The aim of this paper is to interpret quantitatively the experimental results of Challis and Halbo on the basis of the theory proposed by Suzuki and Mikoshiba[2] which takes into account the splittings of the acceptor ground-state quartet into four levels under the influence of magnetic field.

The contributions of elastic and inelastic phonon scatterings by shallow acceptors to the low-temperature magneto-thermal conductivity of Si are calculated in detail. It is shown that in the temperature range 1–5 K and for magnetic fields up to 55 kG, the elastic scattering makes major contributions towards phonon resistivity. We have also tried to explain the experimental results of the reduced thermal conductivity κ/κ_0 of the boron-doped Si specimen at various temperatures as a function of magnetic field H, applied parallel to the specimen axis. The main features of the curves κ/κ_0 vs H are explained in the present paper. Some alternative possibilities are examined for the discrepancies between theory and experiment.

II. THEORY

The ground state of shallow acceptors in Ge and Si has fourfold degeneracy and Γ_8 symmetry. The fourfold-degenerate ground state splits into two Kramer's doublets, $M_J=\pm\frac{3}{2}$ and $\pm\frac{1}{2}$, when the uniaxial stress is applied along the [001] or [111] crystallographic axis. However, in the presence of the magnetic field, the ground state splits into four levels.

The interactions of acceptor holes with the lattice and the magnetic field are represented by the following Hamiltonian[3]:

$$H_{\mathrm{hp}}=\tfrac{2}{3}D_u^a[(J_x^2-\tfrac{1}{3}J^2)e_{xx}+\text{c.p.}] +\tfrac{1}{3}D_{u'}^a[(J_xJ_y+J_yJ_x)e_{xy}+\text{c.p.}]\,, \quad (1)$$

$$H_z=\beta[g\vec{J}\cdot\vec{H}+f(J_x^3H_x+\text{c.p.})]\,. \quad (2)$$

Here D_u^a and $D_{u'}^a$ are the deformation potential constants for the acceptor holes, β is the Bohr magneton, J_α is the αth component of the angular-momentum operator for $J=\frac{3}{2}$, $e_{\alpha\beta}$ is the conventional strain component, c.p. denotes the cyclic permutation with respect to the indices x, y, and z, and H is the magnetic field.

Suzuki and Mikoshiba[2] have given a theory for the magnetic-field dependence of the phonon conductivity of a lightly doped p-type Si and Ge. In the presence of the magnetic field H, the four states $|M_J=+\frac{3}{2}\rangle$, $|M_J=+\frac{1}{2}\rangle$, $|M_J=-\frac{1}{2}\rangle$, and $|M_J=-\frac{3}{2}\rangle$ with different energies are referred to as (for states 1–4, respectively)

$$E(M_J=+\tfrac{3}{2})=g_{3/2}\tfrac{3}{2}\beta H\,,$$

$$E(M_J=+\tfrac{1}{2})=g_{1/2}\tfrac{1}{2}\beta H\,,$$

$$E(M_J=-\tfrac{1}{2})=-g_{1/2}\tfrac{1}{2}\beta H\,,$$

$$E(M_J=-\tfrac{3}{2})=-g_{3/2}\tfrac{3}{2}\beta H\,.$$

The energy difference Δ of the different two-level systems are given by

$$\begin{aligned}\Delta &= \Delta_{12} = \Delta_{34} = \tfrac{1}{2}(3g_{3/2} - g_{1/2})\beta H \,,\\ \Delta &= \Delta_{13} = \Delta_{24} = \tfrac{1}{2}(3g_{3/2} + g_{1/2})\beta H \,,\\ \Delta &= \Delta_{14} = 3g_{3/2}\beta H \,,\\ \Delta &= \Delta_{23} = g_{1/2}\beta H \,.\end{aligned} \tag{3}$$

The phonon-hole scattering relaxation rate is expressed as

$$\tau_{\mathrm{hp}}^{-1}(qj) = \tau_{\mathrm{el}}^{-1}(qj) + \tau_1^{-1}(qj) + \tau_2^{-1}(qj) \,, \tag{4}$$

where $\tau_{\mathrm{el}}^{-1}(qj)$ for a two-level system denotes the relaxation rate due to elastic scattering of phonons both from the upper as well as the lower level, $\tau_1^{-1}(qj)$ represents the relaxation rate due to inelastic scattering of phonons from the upper level, $\tau_2^{-1}(qj)$ represents the relaxation rate due to "thermally assisted" phonon absorption for $\omega_{qj} < \Delta/\hbar$ and inelastic scattering by holes in lower level for $\omega_{qj} > \Delta/\hbar$. Here Δ is the energy difference for the two-level system, which, in the present case, can take values given by $\Delta = \Delta_{12}$, Δ_{13}, Δ_{14}, and Δ_{23}.

The elastic-scattering relaxation rate for the present system is given by

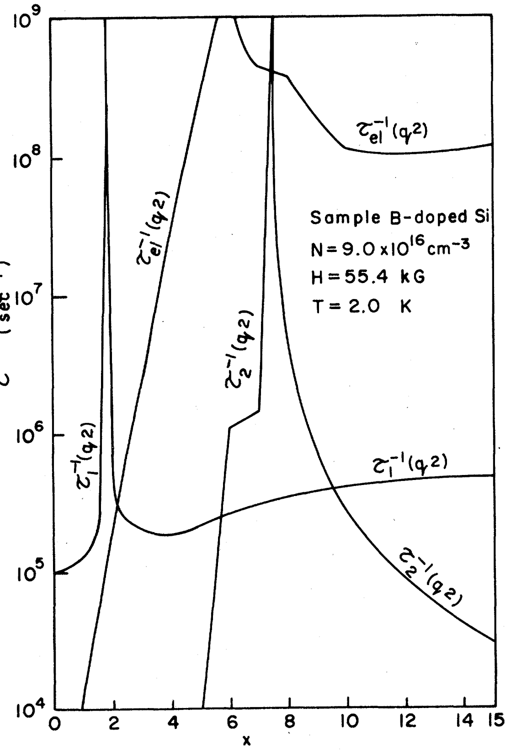

FIG. 1. Various relaxation rates τ^{-1} of phonons versus x in B-doped Si ($N = 9.0 \times 10^{16}$ cm^{-3}) in the presence of the magnetic field, $H = 10$ kG at $T = 2.0$ K. τ_{el}^{-1} is the relaxation rate due to elastic phonon scattering; τ_1^{-1} and τ_2^{-1} are the relaxation rates due to inelastic phonon scattering.

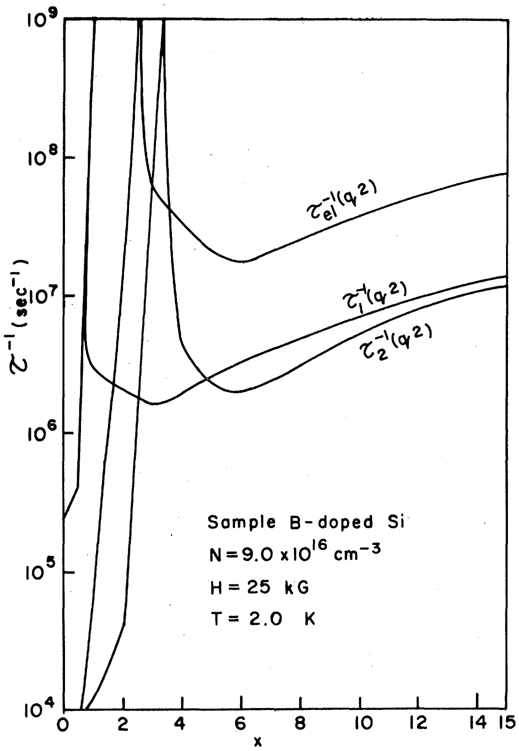

FIG. 2. Various relaxation rates τ^{-1} of phonons versus x in B-doped Si ($N = 9.0 \times 10^{16}$ cm^{-3}) in the presence of the magnetic field, $H = 25$ kG at $T = 2.0$ K. τ_{el}^{-1} is the relaxation rate due to elastic phonon scattering; τ_1^{-1} and τ_2^{-1} are the relaxation rates due to inelastic phonon scattering.

TABLE I. Values of the physical parameters used in the calculation of the magneto-thermal conductivity of boron-doped Si in the temperature range 1–5 K for magnetic fields up to 55.4 kG (Fig. 4) and up to 100 kG (Fig. 3).

Samples	Boron-doped Si
ρ (g/cm^3)	2.33
v_1 (cm/sec)	9.33×10^5
v_2 (cm/sec)	5.42×10^5
N (cm^{-3})	9.0×10^{16}
L (cm)	0.3
A (sec^3)	1.32×10^{-45}
a_0 (Å)	7.0
D_u^a (eV)	2.0
$D_{u'}^a$ (eV)	3.1
β (erg/G)	9.27410×10^{-21}
$g_{1/2}$	0.97 (Fig. 3) 1.00 (Fig. 4)
$g_{3/2}$	1.22 (Fig. 3) 2.33 (Fig. 4)

$$\tau_{el}^{-1}(qj) = \frac{4N(D_{u'}^a)^4 k_B^4 X^4 T^4}{2025\pi\rho^2\hbar^4 v_j^2}\left[1+\left(\frac{a_0 k_B}{2v_j\hbar}\right)^2 x^2T^2\right]^{-4}$$
$$\times\left\{v_1^{-5}\left[1+\left(\frac{a_0k_B}{2v_1\hbar}\right)^2 x^2T^2\right]^{-4} + \tfrac{3}{2}v_2^{-5}\left[1+\left(\frac{a_0k_B}{2v_2\hbar}\right)^2x^2T^2\right]^{-4}\right\}W_j, \quad (5)$$

where

$$W_1 = 8(B_1 + \tfrac{1}{2}B_2 + B_3),$$
$$W_2 = 7B_1 + B_2 + 2B_3, \quad (6)$$
$$W_3 = 5B_1 + 5B_2 + 10B_3,$$

and

$$B_1 = \frac{\Delta_{12}^2 + k_B^2x^2T^2}{(\Delta_{12}^2 - k_B^2x^2T^2)^2},$$
$$B_2 = \frac{\Delta_{13}^2(D^4+1)}{(\Delta_{13}^2 - k_B^2x^2T^2)^2}, \quad (7)$$
$$B_3 = \frac{D^2k_B^2x^2T^2}{(\Delta_{13}^2 - k_B^2x^2T^2)^2},$$

$$D = D_u^a/D_{u'}^a.$$

For the complete expression of the inelastic relaxation rate τ_1^{-1} in the presence of the magnetic

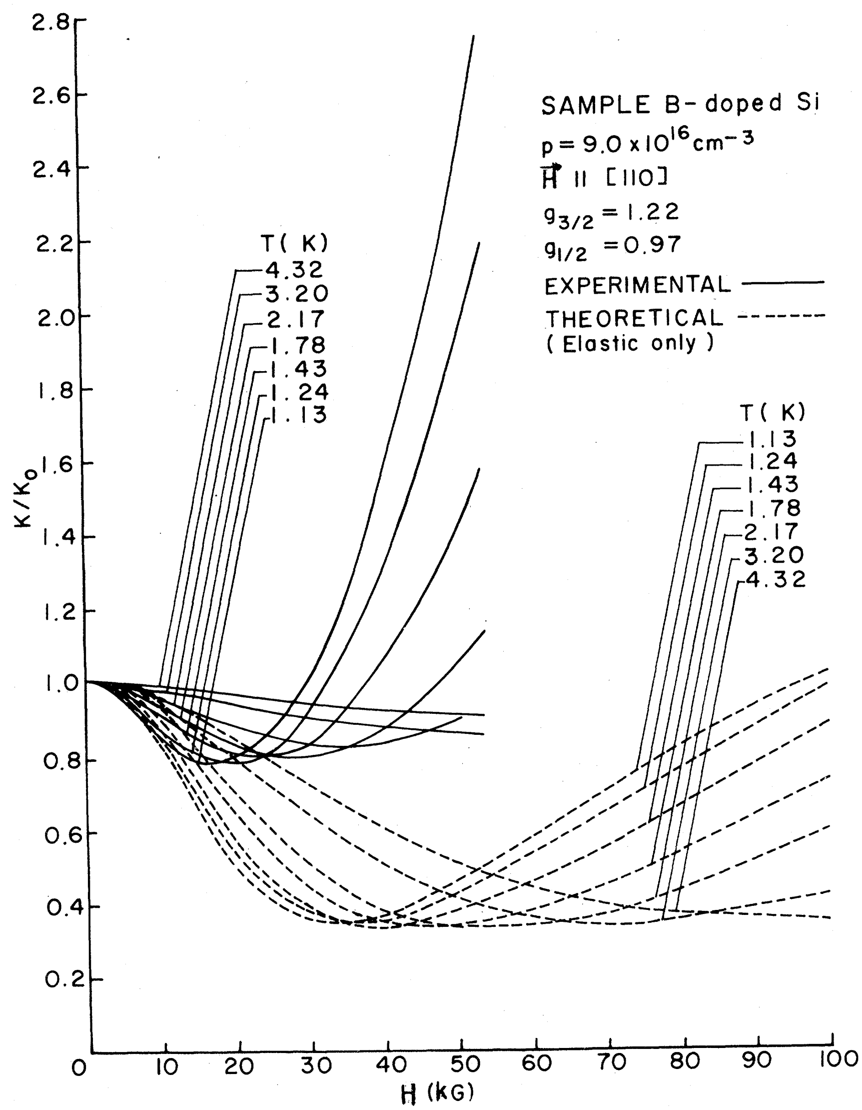

FIG. 3. Variation of reduced phonon conductivity with the magnetic field at different temperatures in B-doped Si ($N = 9.0\times10^{16}$ cm^3) with $g_{3/2} = 1.22$ and $g_{1/2} = 0.97$. Experimental results are shown by solid lines and theoretical results by dotted curves.

field H, the reader may consult the paper of Suzuki and Mikoshiba. The expression for τ_2^{-1} can be written on a similar basis.

III. RESULTS AND DISCUSSION

We have evaluated τ_{e1}^{-1}, τ_1^{-1}, and τ_2^{-1} and plotted them as a function of x for $T = 2.5$ K for two different values of the magnetic field. We find that except for a very narrow range of x, τ_{e1}^{-1} dominates over τ_1^{-1} and τ_2^{-1}; see Figs. 1 and 2.

We have evaluated phonon conductivity of boron-doped Si(B) at different temperatures for magnetic fields varying up to $H = 55.4$ kG applied ∥ to [110] direction. The values of the various parameters used in the present calculations are given in Table I. It has been found that the inelastic contribution is negligible for all the values of magnetic fields over the entire temperature range 1–5 K. It may also be mentioned here that in the present temperature range, the only additional scattering mechanisms which have been considered are the boundary scattering of phonons and point-defect scattering of phonons, which have ω^4 dependence. In order to determine the effective relaxation time, we have assumed the additivity of the reciprocal relaxation times and the phonon conductivity is evaluated in the framework of Callaway's theory.

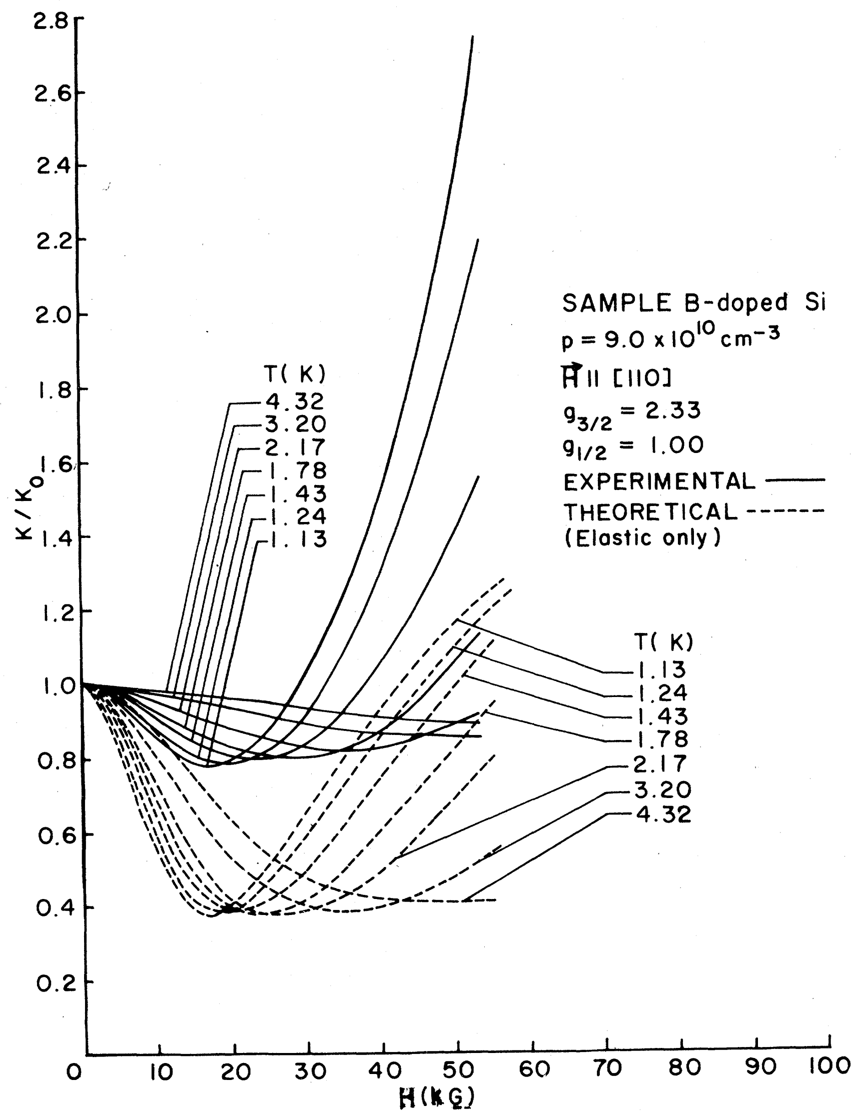

FIG. 4. Variation of reduced phonon conductivity with the magnetic field at different temperatures in B-doped Si ($N = 9.0 \times 10^{16}$ cm^3) with $g_{3/2} = 2.33$ and $g_{1/2} = 1.00$. Experimental results are shown by solid lines and theoretical results by dotted curves.

Figure 3 shows the plot of $\kappa(H)/\kappa(H=0)=\kappa/\kappa_0$ vs H (kG) at different temperatures. The hole concentration is $9\times10^{+16}$ cm^{-3}. Experimentally the situation can be summarized as follows. Except for the two temperatures 4.32 and 3.2 K, for which κ/κ_0 goes on decreasing, this ratio first decreases with the increase in the magnetic field and then increases with the increase in the magnetic field, causing a dip in the ratio κ/κ_0 at a particular value of H. The dip shifts toward lower magnetic fields with the decrease in the temperature. For temperatures 1.78, 1.43, 1.24, and 1.13 K, the ratio κ/κ_0 not only increases rapidly beyond the dip but shoots up to values for which $(\kappa/\kappa_0)>1$. For 1.13 K, the ratio shoots up to 2.7 at 55 kG. The comparison between experiment and theory is shown in Fig. 3. Theoretical results are shown by dotted curves. For Fig. 3 calculations have been done using the theoretical g values,[3] $g_{3/2}=1.22$ and $g_{1/2}=0.97$ for magnetic fields up to 100 kG.

It may be seen from Fig. 3 that the theoretical curves shown by dotted lines reproduce the qualitative features of the experimental results. However, the theoretical plots of $\kappa(H)/\kappa(H=0)$ vs H show the rising tendency for large values of the fields, and the increase in the ratio $\kappa(H)/\kappa(H=0)$ is also not as marked as in the case for the experimental results at lower temperatures. The dips in the curves, i.e., where the minimum occurs in the ratio $\kappa(H)/\kappa(H=0)$, are also located at fields larger than the experimentally observed values. Quantitative agreement between theory and experiment can be improved if we change the values of $g_{3/2}$ and $g_{1/2}$ (see Fig. 4). However, this value of $g_{3/2}$ (=2.33) is much higher than the theoretical value[3] (=1.22) which has recently been substantially confirmed by EPR.[4] It is suggested that the reason for this discrepancy is zero-field splitting of the $|M_J=\pm\frac{3}{2}\rangle$ and $|M_J=\pm\frac{1}{2}\rangle$ states produced by random strains. It has been shown by low-temperature thermal-conductivity measurements by Challis *et al.*[5] that these splittings can be as large as ~30 GHz for Germanium acceptors and this is quite comparable to the relevant field splittings in the region of the minimum. For example at 10 kG, $\Delta_{12}=19$ and $\Delta_{13}=33$ GHz. So if these are comparable splittings in silicon this could explain why the minima occur at lower fields than predicted—the levels are already substantially split—and also why the minima are shallower relative to the zero-field values than predicted.

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