

LETTERS TO THE EDITOR

ROLE OF THREE PHONON NORMAL PROCESSES IN THE PHONON CONDUCTIVITY OF SILICON

IN SPITE OF the fact that some refinements¹⁻⁴ have been proposed recently, the success of the Callaway⁵ theory of the lattice thermal conductivity in explaining the experimental results has been tremendous at

$$K = (k_B/2\pi^2) (k_B T/\hbar)^3 (1/v_s) \int_0^{\theta/T} \frac{x^4 e^x (e^x - 1)^{-2} dx}{v_s/L + Dx^4 + E_1 x^2/(1+a)} \quad \text{for } \tau_N^{-1} < \tau_R^{-1}$$

and for $\tau_N^{-1} > \tau_R^{-1}$ it reduces to

$$K = (k_B/2\pi^2) (k_B T/\hbar)^3 (1/v_s) \left\{ \frac{\left[\int_0^{\theta/T} x^4 e^x (e^x - 1)^{-2} dx \right]^2}{\left[\int_0^{\theta/T} (v_s/L + Dx^4 + E_1 x^2/(1+a)) x^4 e^x (e^x - 1)^{-2} dx \right]} \right\}$$

low temperatures. Using the displaced Planck distribution function, Callaway obtained an expression for the lattice thermal conductivity which can be divided into two parts. The first part gives the lattice thermal conductivity due to the combined scattering relaxation rate while the second part is known as the correction term due to three phonon normal processes. In the recent studies⁶⁻¹⁰, it has been found that the contribution of the correction term due to three phonon normal processes towards the total phonon conductivity can be neglected due to its very small contribution except for solid He¹¹ and LiF¹². Recently Dubey and Verma⁶ studied the role of three phonon normal processes in the phonon conductivity of Ge and it is reported that the Callaway integral gives best result for $\tau_N^{-1} < \tau_R^{-1}$ and for the relative scattering strength of three phonon normal and umklapp processes as 10^{-3} . Following the earlier work of Dubey and Verma, in the present note, we have studied the role of three phonon normal processes in the lattice thermal conductivity of Si in the temperature range of 2-100° K and it is found that the Callaway integral of the lattice thermal conductivity gives best fit between calculated and experimental value of the phonon conductivity for the relative scattering strength of three phonon normal and umklapp processes 'a' = 10^{-3} . It has also been reported that for $\tau_N^{-1} > \tau_R^{-1}$, the Callaway integral of the lattice thermal conductivity not only fails to give

good fit but also leads to a wrong temperature dependence of the phonon conductivity which is similar to the previous report of Dubey and Verma for Ge.

Following the earlier work of Dubey and Verma and considering the Callaway theory, the lattice thermal conductivity of an insulator can be expressed as:

where k_B is the Boltzmann constant, \hbar is the Planck constant divided by 2π , v_s is the average phonon velocity, L is the Casimir length of the crystal, θ is the Debye temperature and E_1 is the three phonon scattering strength. In writing the above stated expression, following scattering relaxation rates have been used.

Boundary scattering relaxation rate $^{13}\tau_B^{-1} = v_s/L$

Point defect scattering relaxation rate $^{14}\tau_{pt}^{-1} = Aw^4$

Three phonon normal processes scattering relaxation rate $\tau_N^{-1} = B_2 w^2 T^3$

Three phonon umklapp processes scattering relaxation rate $\tau_U^{-1} = B_1 w^2 T^3$

Combined three phonon scattering relaxation rate

$\tau_{3ph}^{-1} = (B_1 + B_2) w^2 T^3 = E w^2 T^3 \equiv E_1 x^2$

where B_1 and B_2 are the scattering strengths of three phonon umklapp and normal processes respectively and A is the point defect scattering strength. In the expressions (1) and (2), 'a' means B_2/B_1 and $\tau_R^{-1} = \tau_B^{-1} + \tau_{pt}^{-1} + \tau_U^{-1}$.

The values of the different parameters which have been used in the calculation of the phonon conductivity of Si in the temperature range 2-100° K are listed in Table I. To study the role of normal processes, lattice thermal conductivity has been calculated for the different values of the relative scattering strength of three phonon normal and umklapp processes, i.e., $a = 10^{-3}$ to 10^3 .

TABLE I

The parameters and constants used in the calculation of lattice thermal conductivity of Si to study the role of three phonon normal processes

$\tau_B^{-1} = 2.0 \times 10^6 \text{ sec}^{-1}$
$A = 2.47 \times 10^{-45} \text{ sec}^3$
$E = 3.4 \times 10^{-24} \text{ sec deg}^{-3}$
$v_s = 6.53 \times 10^5 \text{ cm/sec}$
$\theta = 658^\circ \text{ K.}$

For $\tau_N^{-1} < \tau_R^{-1}$, eq. (1) is used to calculate phonon conductivity for the four different values of 'a' (0.001, 0.01, 0.1 and 1.0). Similarly for $\tau_N^{-1} > \tau_R^{-1}$, lattice thermal conductivity is calculated for 'a' = 10, 100, 1,000 using eq. (2). The result is shown in Fig. 1. From Fig. 1, it can be seen that the Callaway theory gives excellent agreement between calculated and experimental results of phonon conductivity of Si for $\tau_N^{-1} < \tau_R^{-1}$ when 'a' is approaching to 10^{-3} . However for $\tau_N^{-1} > \tau_R^{-1}$, the theory fails to yield the correct temperature dependence of the phonon conductivity.

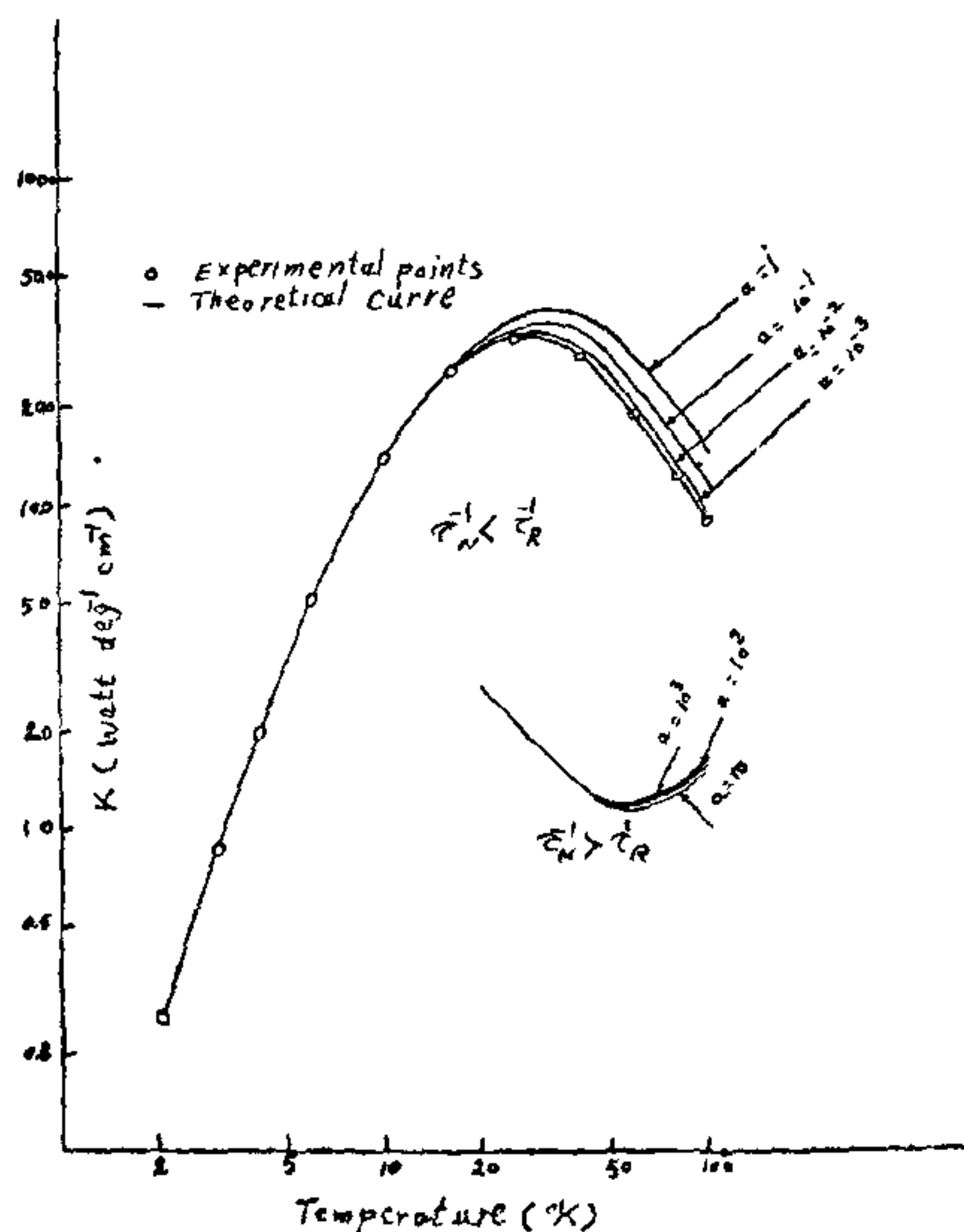


FIG. 1. Phonon conductivity of Si in the temperature range 2-100° K. Solid lines are the calculated value. Circles are the experimental points. 'a' is the relative scattering strength of three phonon normal and umklapp processes.

A Similar result was also reported by Dubey and Verma⁶ for Ge in the temperature range 2-100° K. Thus, one can say that the role of three phonon normal processes is similar in the phonon conductivity of Si and Ge at low temperatures.

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CRYSTAL STRUCTURE OF METAMIZOL

1-PHENYL-2, 3-dimethyl-5-pyrazolone-4-methylamino-methane-sulphonate sodium, $C_{13}H_{16}N_3O_4S$. Na, known variously as metamizol, methampyrazone or novalgine, is a well known pain relieving drug. Here we give a preliminary account of the x-ray analysis of this compound carried out as part of a programme of structural studies on analgesics and their interactions.

The crystals were grown by the slow diffusion of ethanol vapour into an aqueous solution of the compound. The space group and the unit cell dimensions of the crystals were determined from oscillation, Weissenberg and Precession photographs, and the density was measured by flotation in a mixture of benzene and carbon tetrachloride. The density indicated the presence of one water molecule per formula unit. The cell dimensions were subsequently refined on a four circle diffractometer.

Crystal data: Space group $P2_1/c$.

a 9.143(3), b 49.50(2), c 7.314(2) Å;
β 90.2(1); D 1.388 ± 0.005, ρ 1.401 gm/c.c., Z 8.

The intensity data were collected on a Picker four circle diffractometer. The structure was solved by the direct methods and refined isotropically to a