Journal of Thermal Analysis, Vol. 18 (1980) 35–55

ANALYSIS OF THE LATTICE THERMAL CONDUCTIVITIES OF Mg_2Si AND Mg_2Sn IN THE TEMPERATURE RANGE 2–1000 K IN THE FRAME OF THE TWO-MODE CONDUCTION OF PHONONS

K. S. DUBEY

Department of Physics, College of Science, University of Basrah, Basrah, Iraq

(Received December 27, 1978)

The lattice thermal conductivities of Mg_2Si and Mg_2Sn have been analyzed in the entire temperature range 2–1000 K in the frame of the expression for the three-phonon scattering relaxation rate recently proposed by Dubey and Misho, and a very good agreement is found between the calculated and the experimental values of the lattice thermal conductivity in the entire temperature range of the study. The separate contributions due to transverse and longitudinal phonons towards the total lattice thermal conductivity have also been studied by calculating their percentage contributions. The percentage contributions of the three-phonon normal and umklapp process scattering relaxation rates towards the three-phonon scattering relaxation rate have been studied for both Mg_2Si and Mg_2Sn. The percentage contribution of the three-phonon scattering relaxation rate towards the combined scattering relaxation rate has also been studied for transverse as well as for longitudinal phonons, for four different values of the phonon frequencies. The role of the four-phonon processes is also included in the present analysis.

It has been well established that the phonon-phonon scattering relaxation rate plays a very important role in the study of the lattice thermal conductivity of an insulator. Due to the complex structure of the Brillouin zone and the strong temperature-dependence of the phonon distribution function, the three-phonon scattering relaxation rate displays a complicated dependence on the phonon frequency and temperature. As a result, even at present, we lack an exact analytical expression for it. For practical purposes, there is a need to express the scattering relaxation rate by simple relations. Three-phonon scattering processes have been studied by several workers [1–11] and it has been found that they can be divided into two groups: a normal process (N-process) in which momentum is conserved, and an umklapp process (U-process) in which momentum is not conserved. The lattice thermal conductivities of a number of samples have been calculated by several workers [5–25] by using simple expressions for the three-phonon scattering relaxation rates as a function of the phonon frequency and temperature. These expressions are listed in Table 1. However, due to complications, none of the previous workers has included the contributions due to both N and U-processes in the same conductivity integral.

Recently, considering the contributions of both N and U-processes, Dubey and Misho [26] proposed a new expression for the three-phonon scattering relaxation rate:

$$\tau_{3ph}^{-1} = (B_N + B_U e^{-\Theta/\alpha T}) g(w) T^n$$

Table 1

The scattering relaxation rates. In these expressions, B's are constants and are known as the scattering strengths of the respective processes, L is the Casimir length of the crystal, A is the point-defect scattering strength, v is the average phonon velocity, α is a constant, Θ is the Debye temperature and q_{max} is the zone boundary of the first Brillouin zone

Scattering processes	Relaxation rates	
Crystal boundary[a]	$\tau_B^{-1} = v/L$	
Impurities[b]	$\tau_{Pt}^{-1} = Aw^4$	
Three-phonon processes τ_{3ph}^{-1}		
Normal processes[c] (N-processes)	$\tau_{3ph,N}^{-1}$	
Transverse	$\tau_{TN}^{-1} = B_T wT^4$	at low temperatures
Longitudinal	$\tau_{LN}^{-1} = B_L w^2 T^3$	at low temperatures
Transverse	$\tau_{TN}^{-1} = B'_T wT$	at high temperatures
Longitudinal	$\tau_{LN}^{-1} = B'_L w^2 T$	at high temperatures
Umklapp processes (U-processes)	$\tau_{3ph,U}^{-1}$	
Klemens[d]	$\tau_U^{-1} = B_U w^2 T^3 e^{-\Theta/\alpha T}$	at low temperatures
Klemens[e]	$\tau_U^{-1} = B'_U wT^3 e^{-\Theta/\alpha T}$	at low temperatures
Holland[f] (for transverse)	$\tau_U^{-1} = B_{TU} w^2/\sinh(\hbar w/k_B T)$	$\frac{1}{2}q_{max} - q_{max}$
	$\tau_U^{-1} = 0$	$0 - \frac{1}{2}q_{max}$
Callaway[g]	$\tau_U^{-1} = B_U w^2 T^3$	
Klemens[h]	$\tau_U^{-1} = B''_U w^2 T$	at high temperatures
Joshi and Verma[i] (transverse)	$\tau_{3ph,T}^{-1} = B_T wT^m$	$0 - q_{max}$
(longitudinal)	$\tau_{3ph,L}^{-1} = B_L w^2 T^m$	$0 - q_{max}$
SDV[j] (transverse)	$\tau_{3ph,T}^{-1} = B_{T,I} wT^m T_c I^{(T)} e^{-\Theta/\alpha T}$	$0 - q_{max}$
(longitudinal)	$\tau_{3ph,L}^{-1} = B_{L,I} w^2 T^m L_c I^{(T)} e^{-\Theta/\alpha T} + B_{L,II} w^2 T^m L_c II^{(T)} e^{-\Theta/\alpha T}$	$0 - q_{max}$
Four-phonon processes[k]	$\tau_{4ph}^{-1} = Bw^2 T^2$	at high temperatures

[a] — ref. 41, [b] — refs. 4 and 2, [c] — ref. 1, [d] — ref. 3, [e] — ref. 2,
[f] — ref. 6, [g] — ref. 5, [h] — ref. 2, [i] — ref. 11, [j] — refs. 8–10
[k] — refs. 30–32

and is found [26–29] that this gives a good response to the experimental lattice thermal conductivity data. The terms are explained in the following section. The aim of the present work is to calculate the lattice thermal conductivities of Mg_2Si and Mg_2Sn in the temperature range 2–1000 K in the frame of the expression for the three-phonon scattering relaxation rate proposed by Dubey and Misho [26] as stated above. The separate contributions of transverse and longitudinal phonons towards the total lattice thermal conductivities of Mg_2Si and Mg_2Sn have also been studied by calculating their percentage contributions. The percentage contributions of the three-phonon N and U-process scattering relaxation rates towards the three-phonon scattering relaxation rate τ_{3ph}^{-1} have been studied for both samples. The percentage contribution of τ_{3rh}^{-1} towards the combined scattering relaxation rate has also been studied for four different values of the phonon frequencies for both modes, transverse and longitudinal phonons, and also for Mg_2Si as well as Mg_2Sn.

The contribution of the four-phonon scattering processes [30–32] towards the total lattice thermal resistivity is also included at high temperatures in both of the samples.

A short feature of the Dubey and Hisho approach to lattice thermal conductivity

The phonon-phonon scattering processes dominate over other scattering processes at high temperatures and are not negligibly small at low temperatures. They play an important role even in the vicinity of conductivity maxima. However, it is difficult to express the three-phonon scattering relaxation rate τ_{3ph}^{-1} by a simple relation, due to the complicated structure of the Brillouin zone and the strong temperature-dependence of the phonon distribution function. Several expressions have been proposed for the three-phonon scattering relaxation rate for N and U-processes as a simple function of the phonon frequency w and temperature T; these are reported in Table 1. It is clear from Table 1 that the scattering relaxation rate is different for transverse and longitudinal phonons. The frequency-dependence of τ_{3ph}^{-1} is w for transverse phonons and w^2 for longitudinal phonons. The Callaway expression is an exception, due to the fact that he does not make any distinction between transverse and longitudinal phonons. From Table 1, it is also clear that the expression for τ_{3ph}^{-1} for U-processes contains an exponential factor.

Using these scattering relaxation rates, several workers [5–25, 33–40] have calculated the lattice thermal conductivity for different samples. The expressions they used for the combined scattering relaxation rates are reported in Table 2. From Table 2, it is clear that, due to the complicated role of N and U-processes, none of them has included the contribution due to both processes in the same conductivity integral, i.e. they have used either $\tau_{3ph,N}^{-1}$ or $\tau_{3ph,U}^{-1}$ in one conductivity integral to calculate the lattice thermal conductivity of a sample. From Table 1, it is clear that the three-phonon scattering relaxation rates $\tau_{3ph,N}^{-1}$ and $\tau_{3ph,U}^{-1}$ for N and U-processes, respectively, can be expressed as

$$\tau_{3ph,N}^{-1} = B_N\, g(w)\, T^m \tag{1}$$

$$\tau_{3ph,U}^{-1} = B_U\, g(w)\, T^m\, e^{-\Theta/\alpha T} \tag{2}$$

where B_N and B_U are the scattering strengths due to the respective processes, $g(w)$ represents the frequency-dependence of the three-phonon scattering relaxation rates, which is w for transverse phonons and w^2 for longitudinal phonons, Θ is the Debye temperature of the specimen under study, α is a constant and m is the temperature exponent of the scattering relaxation rates. The same value of m has been assigned to both processes by Dubey and Misho, due to the fact that the Guthrie calculations [7] show equal values of m for N and U-processes and it can be calculated with the help of the Guthrie expression. Thus, the combined scat-

Table 2

The combined scattering relaxation rates. In these expressions, w_1 and w_2 are the transverse phonon frequencies at $\frac{1}{2}q_{max}$ and q_{max}, respectively, w_3 and w_4 are the same for longitudinal phonons, w_D is the Debye frequency and other terms have the same meanings as stated in Table 1

	Combined scattering relaxation rates	Frequency range
Callaway[a]	$\tau_c^{-1} = \tau_B^{-1} + \tau_{pt}^{-1} + (B_1 + B_2)w^2T^3$	$0 - w_D$
Holland[b]	$\tau_{c,T}^{-1} = \tau_B^{-1} + \tau_{pt}^{-1} + B_{TU}wT^4$	$0 - w_1$
	$\tau_{c,T}^{-1} = \tau_B^{-1} + \tau_{pt}^{-1} + B_{TU}w^2/\sinh(\hbar w/k_BT)$	$w_1 - w_2$
	$\tau_{c,L}^{-1} = \tau_B^{-1} + \tau_{pt}^{-1} + B_Lw^2T^3$	$0 - w_4$
Joshi and	$\tau_{c,T}^{-1} = \tau_B^{-1} + \tau_{pt}^{-1} + B_TwT^m$	$0 - w_2$
Verma[c]	$\tau_{c,L}^{-1} = \tau_B^{-1} + \tau_{pt}^{-1} + B_Lw^2T^m$	$0 - w_4$
	(m = 1, 2, 3 and 4, depending on the temperature range)	
SDV model[d]	$\tau_{c,T}^{-1} = \tau_B^{-1} + \tau_{pt}^{-1} + B_{T,I}wT^mT_c I^{(T)}e^{-\Theta/\alpha T}$	$0 - w_2$
	$\tau_{c,L}^{-1} = \tau_B^{-1} + \tau_{pt}^{-1} + B_{L,I}w^2T^mL_cI^{(T)}e^{-\Theta/\alpha T}$	
	$+ B_{L,II}w^2T^mL_cII^{(T)}e^{-\Theta/\alpha T}$	$0 - w_4$
Dubey and	$\tau_{c,T}^{-1} = \tau_B^{-1} + \tau_{pt}^{-1} + (B_{TN} + B_{TU}e^{-\Theta/\alpha T})wT^m$	$0 - w_2$
Misho[e]	$\tau_{c,L}^{-1} = \tau_B^{-1} + \tau_p^{-1} + (B_{LN} + B_{LU}e^{-\Theta/\alpha T})w^2T^m$	$0 - w_4$
(present work)		
	($m = 1-4$ for transverse phonons and $1-3$ for longitudinal phonons, depending on the temperature range.)	

[a] — ref. 5.
[b] — ref. 6.
[c] — ref. 11.
[d] — refs. 8—10.
[e] — refs. 26—28.

tering relaxation rate for τ_{3ph}^{-1} can be expressed [26] as

$$\tau_{3ph}^{-1} = \tau_{3ph,N}^{-1} + \tau_{3ph,U}^{-1} = (B_N + B_U e^{-\Theta/\alpha T})\, g(w)\, T^m \tag{3}$$

Therefore, the combined scattering relaxation rate $\tau_{c,T}^{-1}$ for transverse phonons is given [26] by

$$\tau_{c,T}^{-1} = \tau_B^{-1} + \tau_{pt}^{-1} + (B_{TN} + B_{TU}\, e^{-\Theta/\alpha T})\, wT^m \tag{4}$$

and for longitudinal phonons by

$$\tau_{c,L}^{-1} = \tau_B^{-1} + \tau_{pt}^{-1} + (B_{LN} + B_{LU}e^{-\Theta/\alpha T})w^2T^m \tag{5}$$

where τ_B^{-1} and τ_{pt}^{-1} are the scattering relaxation rates due to boundary [41] walls of the crystal and point-defect [4], respectively, and the expressions for these scattering relaxation rates are those of Casimir [41] and Klemens [4], respectively, listed in Table 1. Suffixes T and L represent transverse and longitudinal phonons, respectively.

The complete separate expression for transverse and longitudinal phonons for the combined scattering relaxation rates, which have been used in the present analysis, are reported in Tables 3 and 7 for Mg_2Si and Mg_2Sn, respectively.

The value of m varies from 1 to 4 for transverse phonons and 1 to 3 for longitudinal phonons, corresponding to the different temperature ranges. The complete expressions for τ_{3ph}^{-1} and τ_c^{-1} used in the present analysis of the lattice thermal conductivities of Mg_2Si and Mg_2Sn are reported in Tables 3 and 7, together with the temperature ranges. In these Tables, it is found that different values of the three-phonon scattering strengths have been used in the different temperature ranges. However, these scattering strengths (B's) are related to each other by temperature, as suggested by Joshi and Verma [11]. Thus, in the new approach of Dubey and Misho, only one adjustable parameter has been used for the three-phonon scattering strength, similarly as in the previous analysis.

Besides the three-phonon scattering processes, four-phonon processes [30–32] also play an important role in the calculation of the lattice thermal conductivity of an insulator at high temperatures. According to Pomeranchuk [30–32], the four-phonon scattering relaxation rate is given by

$$\tau_{4ph}^{-1} = B_H w^2 T^2 \tag{6}$$

where B is the four-phonon scattering strength. Thus, the combined scattering relaxation rate in the presence of the four-phonon scattering processes can be expressed as

$$\tau_c^{-1} = \tau_B^{-1} + \tau_{pt}^{-1} + \tau_{3ph}^{-1} + \tau_{4ph}^{1} \tag{7}$$

Considering the spherical symmetry of the Brillouin zone (i.e. out of three polarization branches one is longitudinal and two are transverse) and the fact that each phonon contributes separately towards the total lattice thermal conductivity, the contribution of each mode of phonons can be expressed [26] as

$$K_i = (1/6\pi^2) \int \tau_{c,i}\, v_{g,i}^2 (\hbar^2 w^2/k_B T^2) \exp(\pi w/k_B T) (\exp(\hbar w/k_B T) - 1)^{-2} q^2\, dq + \Delta K \tag{8}$$

where integration is performed over the first Brillouin zone, $v_{g,i}$ is the group velocity corresponding to the polarization branches under study, q is the phonon wave vector corresponding to the phonon frequency w, k_B is the Boltzmann constant, $\hbar$ is the Planck constant divided by 2π, $\tau_{c,i}$ is the combined scattering relaxation time and i represents the polarization branches of phonons under study. The term ΔK is known as the correction term [5] due to the three-phonon normal processes; it reduces to zero in the absence of the three-phonon normal processes. It has been studied by a number of workers [42–52] and it is found that the contribution of ΔK towards the total lattice thermal conductivity is very small [42–

Table 3

Combined scattering relaxation rates used in the analysis of the lattice thermal conductivity of Mg_2Si

Expressions	Temperature range
Combined scattering relaxation rates for transverse phonons $\tau_{c,T}^{-1}$	
$(\tau_B^{-1})^L + Aw^4 + (B_{TN} + B_{TU}\, e^{-\Theta/\alpha T})wT^4 + B_{HT}w^2T^2$	$T < 80$
$(\tau_B^{-1})^L + Aw^4 + (B_{TN1} + B_{TU1}e^{-\Theta/\alpha T})wT^3 + B_{HT}w^2T^2$	$80 < T < 103$
$(\tau_B^{-1})_T + Aw^4 + (B_{TN2} + B_{TU2}e^{-\Theta/\alpha T})wT^2 + B_{HT}w^2T^2$	$103 < T < 150$
$(\tau_B^{-1})_T + Aw^4 + (B_{TN3} + B_{TU3}e^{-\Theta/\alpha T})wT + B_{HT}w^2T^2$	$T < 150$
Combined scattering relaxation rates for longitudinal phonons $\tau_{c,L}^{-1}$	
$(\tau_B^{-1})_L + Aw^4 + (B_{LN} + B_{LU}\, e^{-\Theta/\alpha T})w^2T^3 + B_{HL}w^2T^2$	$T < 103$
$(\tau_B^{-1})_L + Aw^4 + (B_{LN1} + B_{LU1}e^{-\Theta/\alpha T})w^2T^2 + B_{HL}w^2T^2$	$103 < T < 150$
$(\tau_B^{-1})_L + Aw^4 + (B_{LN2} + B_{LU2}e^{-\Theta/\alpha T})w^2T + B_{HL}w^2T^2$	$T < 150$
The three-phonon scattering strengths (B's) are related to each other as[a]	
$B_{TX1} = 80B_{TX}$ $\quad B_{LX1} = 103B_{LX}$ $B_{TX2} = 103B_{TX1}$ $\quad B_{LX2} = 150B_{LX1}$ $B_{TX3} = 150B_{TX2}$ where X stands for N and U. B_N and B_U are related by[b] $B_{YN} = B_{YU} \exp(-\Theta/\alpha T)$, where $T = 300$ K and Y stands for T and L	

[a] — ref. 11.
[b] — refs. 26—28.

49] in the frame of the Callaway [5] integral, as well as in the frame of the generalized [53—55] Callaway integral at low and at high temperatures, and one can neglect its contribution compared to the contribution due to the first part in Eq. (8). Solid He [50], LiF [51] and solid HD [52] are exceptions to this.

Following Verma et al. [56], Dubey and Misho [26] used a better relation $q = (w/v)(1 + rw^2)$ to express q in terms of w in the above integral, where r is a constant which depends on the dispersion curve of the sample; it can be calculated with the help of the experimental dispersion curve. Thus, the total lattice thermal conductivity can be expressed as

$$K = K_T + K_L \tag{9}$$

where K_T and K_L are the contributions due to transverse and longitudinal phonons, respectively, these contributions being given by

$$K_T = (C/v_{T1}) \int_0^{\Theta_1/T} \tau_{c,T} x^4 e^x (e^x - 1)^{-2} (1 + R_1 x^2)^2 (1 + 3R_1 x^2)^{-1} \, dx +$$

$$+ (C/v_{T2}) \int_{\Theta_1/T}^{\Theta_2/T} \tau_{c,T} x^4 e^x (e^x - 1)^{-2} (1 + R_2 x^2)^2 (1 + 3R_2 x^2)^{-1} \, dx \qquad (10)$$

$$K_L = (C_1/v_{L1}) \int_0^{\Theta_3/T} \tau_{c,L} x^4 e^x (e^x - 1)^{-2} (1 + R_3 x^2)^2 (1 + 3R_3 x^2)^{-1} \, dx +$$

$$+ (C_1/v_{L2}) \int_{\Theta_3/T}^{\Theta_4/T} \tau_{c,L} x^4 e^x (e^x - 1)^{-2} (1 + R_4 x^2)^2 (1 + 3R_4 x^2)^{-1} \, dx \qquad (11)$$

where $C = 2C_1 = (k_B/3\hbar^2)(k_B T/\hbar)^3$, $R_n = r_n(k_B T/\hbar)^2$, $\Theta_n = (\hbar w_n/k_B)$, $x = (\hbar w/k_B T)$ and $n = 1, 2, 3$ and 4, v_{T1} and v_{T2} are the transverse phonon velocities in the range $0 - 1/2\, q_{max}$ and $1/2\, q_{max} - q_{max}$, respectively, v_{L1} and v_{L2} are the same for longitudinal phonons, w_1 and w_2 are the transverse phonon frequencies corresponding to the phonon wave vector $1/2\, q_{max}$ and q_{max}, respectively, w_3 and w_4 are the same for longitudinal phonons, q_{max} corresponds to the zone boundary of the first Brillouin zone, r_1 and r_2 are the dispersion constants for transverse phonons in the ranges $0 - 1/2\, q_{max}$ and $1/2\, q_{max} - q_{max}$, respectively, and r_3 and r_4 are the same for longitudinal phonons.

Lattice thermal conductivity of Mg_2Si

The constants relating to the dispersion curve are calculated with the help of the experimental dispersion curve measured by Whitten et al. [57]. It is known that at very low temperature the entire lattice thermal resistivity is due to the boundary scattering alone, and one can calculate the Casimir [41] length of the crystal at such temperature. Thus, $(\tau_B^{-1})_T$ and $(\tau_B^{-1})_L$ are calculated at 4 °K with the help of the Casimir length of the crystal. From the values of these two constants, the point-defect scattering strength A has been calculated at 6 K. The value of the temperature exponent m has been calculated with the help of the Guthrie expression (see Eq. (17) of ref. 7).

As far as the three-phonon scattering strengths are concerned, they involve complications due to the fact that both N and U-processes are included in the same conductivity integral in the present study. From the earlier reports of the previous workers, it is clear that $\tau_{3ph\,N}^{-1}$ dominates over $\tau_{3ph,U}^{-1}$ at low temperatures. Keeping in view the above fact and ignoring the contribution of $\tau_{3ph,U}^{-1}$ towards the combined scattering relaxation rate, B_{TN} and B_{LN} have been calculated at 20 K (near the conductivity maxima). It has also been found that at high temperatures, $\tau_{3ph,U}^{-1}$ dominates over $\tau_{3ph,N}^{-1}$. Therefore, Dubey and Misho assumed

equal contributions due to these two processes at room temperature. Thus, following Dubey and Misho [26], using the relation $\tau_{3ph,N}^{-1} = \tau_{3ph,U}^{-1}$ at $T = 300$ K and including the contribution due to three-phonon umklapp processes too, B_{TN} and B_{LN} are finally calculated at 20 K by numerical integration of the conductivity integrals given in the previous section.

Table 4

The constants used in the analysis of the lattice thermal conductivities of Mg_2Si and Mg_2Sn in the entire temperature range 2–1000 K

Constants		Mg_2Si	Mg_2Sn
v_{T1}	(cm sec^{-1})	$4.60 \cdot 10^5$	$3.19 \cdot 10^5$
v_{T2}	(cm sec^{-1})	$1.40 \cdot 10^5$	$1.16 \cdot 10^5$
v_{L1}	(cm sec^{-1})	$6.40 \cdot 10^5$	$4.30 \cdot 10^5$
v_{L2}	(cm sec^{-1})	$5.10 \cdot 10^5$	$2.05 \cdot 10^5$
Θ_1	(°K)	154	90
Θ_2	(°K)	224	118
Θ_3	(°K)	254	138
Θ_4	(°K)	392	176
Θ/α	(°K)	250	225
r_1	(sec^2)	$3.250 \cdot 10^{-28}$	$1.788 \cdot 10^{-27}$
r_2	(sec^2)	$6.428 \cdot 10^{-28}$	$3.776 \cdot 10^{-27}$
r_3	(sec^2)	$1.019 \cdot 10^{-29}$	$3.363 \cdot 10^{-28}$
r_4	(sec$_2$)	$8.804 \cdot 10^{-29}$	$1.388 \cdot 10^{-27}$
$(\tau_B^{-1})_T$	(sec^{-1})	$5.68 \cdot 10^5$	$1.21 \cdot 10^6$
$(\tau_B^{-1})_L$	(sec^{-1})	$7.90 \cdot 10^5$	$1.21 \cdot 10^6$
A	(sec^3)	$8.0 \cdot 10^{-46}$	$1.6 \cdot 10^{-44}$
B_{TN}	(deg^{-4})	$1.12 \cdot 10^{-11}$	$4.77 \cdot 10^{-11}$
B_{LN}	(sec deg^{-3})	$1.20 \cdot 10^{-22}$	$7.20 \cdot 10^{-22}$
B_{HT}	(sec deg^{-2})	$2.0 \cdot 10^{-23}$	$6.0 \cdot 10^{-22}$
B_{HL}	(sec deg^{-2})	$2.0 \cdot 10^{-23}$	$6.0 \cdot 10^{-22}$
r_0	(Å)	—	40
4Δ	(eV)	—	$5.0 \cdot 10^{-4}$
ϱ	(g cm^{-3})	—	3.592
η_{ex}		—	$2.4 \cdot 10^{-16}$
H	(sec^{-1}deg^{-2})	—	$2.7 \cdot 10^6$

From the three-phonon scattering strengths, the lattice thermal conductivity has been calculated and it has been found that the calculated value of the lattice thermal resistivity is lower than the experimental value; this is due to the contribution of the four-phonon processes. Thus, the four-phonon scattering strengths B_{HT} and B_{HL} are adjusted at 300 K.

From all the constants reported in Table 4 and the combined scattering relaxation rates in Table 3, the total lattice thermal conductivity of Mg_2Si has been calculated in the entire temperature range 2–1000 K by calculating separate contributions due to transverse and longitudinal phonons with the help of numerical integration of the conductivity integrals given in Eqs. (10 and (11), and the

result obtained is shown in Fig. 1. The percentage contributions of transverse and longitudinal phonons towards the total lattice thermal conductivity have also been calculated, and the results obtained are shown in Fig. 2. To study the roles of three-phonon N and U-processes, the percentage contributions due to the three-phonon normal process scattering relaxation rate ($\%\tau^{-1}_{3\text{ph N}}$) and the three-phonon umklapp process scattering relaxation rate ($\%\tau^{-1}_{3\text{ph,U}}$) towards $\tau^{-1}_{3\text{ph}}$ have been calculated in the entire temperature range of study, and the results obtained are shown in Fig. 3. The percentage contribution of the three-phonon scattering re-

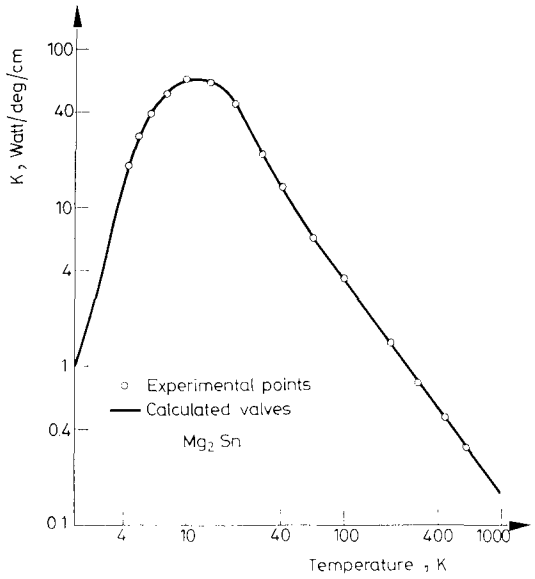

Fig. 1. The total lattice thermal conductivity of Mg_2Si in the temperature range 2–1000 K. The solid line represents the calculated values, and circles are the experimental points

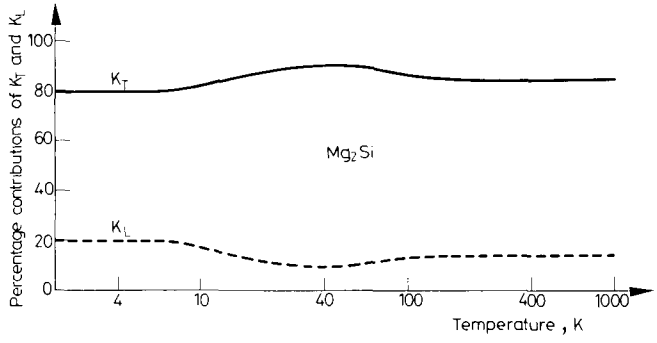

Fig. 2. The percentage contributions due to transverse and longitudinal phonons towards the total lattice thermal conductivity of Mg_2Si. The solid line represents the percentage contribution due to transverse phonons, while the dotted line is that due to longitudinal phonons

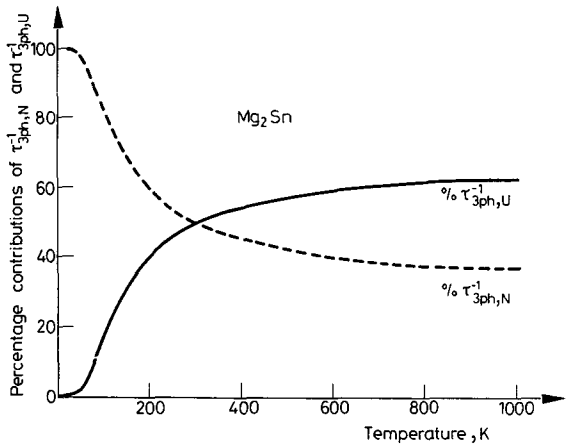

Fig. 3. The percentage contributions due to three-phonon N and U-process scattering relaxation rates towards τ^{-1}_{3ph} for Mg_2Si. The dotted line is the percentage contribution due to the three-phonon normal process scattering relaxation rate ($\%\tau^{-1}_{3ph,N}$), and the solid line is that due to three-phonon umklapp processes

Table 5

The percentage contribution of the three-phonon scattering relaxation rate $\tau^{-1}_{3ph,T}$ towards the combined scattering relaxation rate $\tau^{-1}_{c,T}$ for transverse phonons for Mg_2Si in the absence of four-phonon processes, for four different values of the phonon frequencies. w_{max} is the maximum frequency of the transverse phonons

T, K	% $\tau^{-1}_{3ph,T}$ for $w = \frac{1}{4}w_{max}$	% $\tau^{-1}_{3ph,T}$ for $w = 1/2w_{max}$	% $\tau^{-1}_{3ph,T}$ for $w = 3/4w_{max}$	% $\tau^{-1}_{3ph,T}$ for $w = w_{max}$
1000	99.997	99.992	99.977	99.947
900	99.997	99.991	99.974	99.940
800	99.996	99.990	99.970	99.922
700	99.996	99.988	99.965	99.920
600	99.995	99.986	99.958	99.903
500	99.993	99.982	99.947	99.877
400	99.991	99.976	99.929	99.835
300	99.987	99.965	99.894	99.755
200	99.976	99.937	99.809	99.599
100	99.900	99.728	99.183	98.124
90	99.854	99.612	98.839	97.344
80	99.785	99.427	98.293	96.124
70	99.621	98.994	97.028	93.358
60	99.280	98.102	94.488	88.068
50	98.490	98.068	89.018	77.728
40	96.353	90.825	76.658	58.574
30	89.279	75.729	50.862	30.827
20	62.179	38.118	16.968	8.087
10	9.318	3.707	1.261	0.547
8	4.039	1.552	0.520	0.224
6	1.314	0.496	0.165	0.071
4	0.262	0.098	0.032	0.014
2	0.016	0.006	0.004	0

Table 6

The percentage contribution of the three-phonon scattering relaxation rate $\tau_{3ph,L}^{-1}$ towards the combined scattering relaxation rate $\tau_{c,L}^{-1}$ for longitudinal phonons for Mg_2Si in the absence of four-phonon processes, for four different values of the phonon frequencies. w_{max} is the maximum frequency of the longitudinal phonons

T, K	% $\tau_{3ph,L}^{-1}$ for $w = 1/4 w_{max}$	% $\tau_{3ph,L}^{-1}$ for $w = 1/2 w_{max}$	% $\tau_{3ph,L}^{-1}$ for $w = 3/4 w_{max}$	% $\tau_{3ph,L}^{-1}$ for $w = w_{max}$
1000	99.997	99.990	99.977	99.959
900	99.996	99.988	99.974	99.914
800	99.995	99.986	99.970	99.947
700	99.995	99.984	99.965	99.938
600	99.994	99.981	99.957	99.925
500	99.992	99.976	99.946	99.905
400	99.989	99.967	99.928	99.873
300	99.984	99.952	99.893	99.811
200	99.971	99.913	99.807	99.658
100	99.874	99.624	99.172	98.543
90	99.821	99.464	98.823	97.934
80	99.735	99.210	98.272	96.976
70	99.592	98.786	97.355	95.407
60	99.335	98.033	95.754	92.713
50	98.834	96.584	92.751	87.834
40	97.724	93.427	86.631	78.523
30	94.749	85.750	78.110	60.575
20	84.234	64.055	44.642	31.272
10	40.043	18.217	9.157	5.381
8	25.482	10.237	4.908	2.830
6	12.607	4.590	2.131	1.214
4	4.099	1.406	0.641	0.363
2	0.531	0.178	0.081	0.045

laxation rate $\%\tau_{3ph}^{-1}$ towards the combined scattering relaxation rate τ_c^{-1} has been studied in the entire temperature range 2 – 1000 K in the absence of four-phonon scattering processes, for the four different values of the phonon frequencies $w = 1/4\, w_{max}$, $1/2\, w_{max}$, $3/4\, w_{max}$ and w_{max}, for transverse as well as for longitudinal phonons, to examine the dominating nature of τ_{3ph}^{-1} over τ_B^{-1} and τ_{pt}^{-1}, and the results obtained are reported in Tables 5 and 6, where w_{max} is the maximum phonon frequency in the first Brillouin zone corresponding to the phonon modes under study.

Lattice thermal conductivity of Mg_2Sn

The sample of Mg_2Sn taken in the present analysis displayed neutral donor scattering, as predicted by Martin and Denielson [58]. Therefore, before the detail of calculations, it is necessary to give a short account of the resonant phonon

scattering mechanism which has been introduced in the analysis of the lattice thermal conductivity of Mg_2Sn as an extra scattering mechanism, unlike that of Mg_2Si; it plays a very important role in the calculation of the lattice thermal conductivity of the present sample at low temperatures. Martin and Denielson [58] used the w^4 dependence for the resonant phonon scattering relaxation rate τ_r^{-1}, which is not valid for $\hbar w \gg 4\Delta$ and $k_B T \gg 4\Delta$ in their previous study; 4Δ is the energy separation between the ground state and next higher energy state. The resonant scattering relaxation rate has been studied by different workers [59–63]. In the present work, the modified expression of Kumar and Verma [64] for τ_r^{-1} has been used to analyse the lattice thermal conductivity of Mg_2Sn. According to the modified expression of Kumar and Verma [64], the resonant phonon scattering relaxation rate can be expressed as

$$\tau_r^{-1} = \tau_r^{-1}\,(\text{elastic}) + \tau_r^{-1}\,(\text{inelastic}) \tag{12}$$

$$\tau_r^{-1}\,(\text{elastic}) = H_1' F^4(q) w^2 [f_0(T)(\hbar w/k_B T)^2 + f(T)] \quad \text{for } \hbar w \ll 4\Delta \tag{13}$$

$$\tau_r^{-1}\,(\text{inelastic}) = H_1'' F^4(q)(4\Delta/k_B T)(4\Delta/\hbar)^3 f(T) \quad \text{for } \hbar w \ll 4\Delta \tag{14}$$

$$\tau_r^{-1}\,(\text{elastic}) = H_2' F^4(q) w^2 [f_0(T) + f(T)] \quad \text{for } \hbar w \gg 4\Delta \tag{15}$$

$$\tau_r^{-1}\,(\text{inelastic}) = H_2'' F^4(q) w^2 [f_0(T) + f(T)] \quad \text{for } \hbar w \gg 4\Delta \tag{16}$$

where τ_r^{-1} (elastic) and τ_r^{-1} (inelastic) are the scattering relaxation rates due to elastic and inelastic resonant phonon scattering processes, respectively, $f_0(T)$ and $f(T)$ are the populations of the ground state and next higher energy state, respectively, and $F(q)$ is known as the form factor, which is given by

$$F(q) = (1 + r_0^2 w^2/4v^2)^{-2} \tag{17}$$

where r_0 is the average radius of the donor orbit. Since our interests lie in the region $\hbar w \gg 4\Delta$, we are not concerned with Eqs. (13) and (14). Thus, following Eq. (12), the resonant phonon scattering relaxation rate τ_r^{-1} corresponding to $\hbar w \gg 4\Delta$ can be expressed as

$$\tau_r^{-1} = H_2 F^4(q) w^2 [f_0(T) + f(T)] \tag{18}$$

where $H_2 = H_2' + H_2''$; H_2 is proportional to the 4$^{\text{th}}$ power of the shear deformation potential, and also contains some terms related to the band structure of the sample under study. In the lack of such data, H_2 is taken as an adjustable parameter. If Eq. (18) is expressed in terms of a dimensionless parameter ($x = \hbar w/k_B T$), it reduces to

$$\tau_r^{-1} = H(1 + \delta x^2)^{-8} x^2 \tag{19}$$

where $H = H_2[f_0(T) + f(T)](k_B T/\hbar)^2$ and $\delta = (r_0^2/4v^2)(k_B T/\hbar)^2$. Thus, the combined scattering relaxation rate used in the present analysis of the lattice thermal

conductivity of Mg_2Sn can be expressed as

$$\tau_c^{-1} = \tau_B^{-1} + \tau_{pt}^{-1} + \tau_r^{-1} + \tau_{3ph}^{-1} + \tau_{4ph}^{-1} \quad (20)$$

and its complete form is given in Table 7.

Table 7

Combined scattering relaxation rates used in the analysis of the lattice thermal conductivity of Mg_2Sn

Expressions	Temperature ranges
Combined scattering relaxation rates for transverse phonons $\tau_{c,T}^{-1}$	
$\tau_B^{-1} + Aw^4 + Hx^2(1+\delta x^2)^{-8} + (B_{TN} + B_{TU}\, e^{-\Theta/\alpha T})wT^4 + B_{HT}w^2T^2$	$T < 36$
$\tau_B^{-1} + Aw^4 + Hx^2(1+\delta x^2)^{-8} + (B_{TN1} + B_{TU1}e^{-\Theta/\alpha T})wT^3 + B_{HT}w^2T^2$	$36 < T < 46$
$\tau_B^{-1} + Aw^4 + Hx^2(1+\delta x^2)^{-8} + (B_{TN2} + B_{TU2}e^{-\Theta/\alpha T})wT^2 + B_{HT}w^2T^2$	$46 < T < 68$
$\tau_B^{-1} + Aw^4 + Hx^2(1+\delta x^2)^{-8} + (B_{TN3} + B_{TU3}e^{-\Theta/\alpha T})wT + B_{HT}w^2T^2$	$T < 68$
Combined scattering relaxation rates for longitudinal phonons $\tau_{c,T}^{-1}$	
$\tau_B^{-1} + Aw^4 + Hx^2(1+\delta x^2)^{-8} + (B_{LN} + B_{LU}\, e^{-\Theta/\alpha T})w^2T^3 + B_{HL}w^2T^2$	$T < 46$
$\tau_B^{-1} + Aw^4 + Hx^2(1+\delta x^2)^{-8} + (B_{LN1} + B_{LU1}e^{-\Theta/\alpha T})w^2T^2 + B_{HL}w^2T^2$	$46 < T < 68$
$\tau_B^{-1} + Aw^4 + Hx^2(1+\delta x^2)^{-8} + (B_{LN2} + B_{LU2}e^{-\Theta/\alpha T})w^2T + B_{HL}w^2T^2$	$T < 68$
The three-phonon scattering strengths (B's) are related to each other as[a]	
$B_{TX1} = 36B_{TX}$ $\quad B_{LX1} = 46B_{LX}$ $B_{TX2} = 46B_{TX1}$ $\quad B_{LX2} = 68B_{LX1}$ $B_{TX3} = 68B_{TX2}$ where X stands for N and U. B_N and B_U are related by[b] $B_{YN} = B_{YU} \exp(-\Theta/\alpha T)$, where $T = 300$ K and Y stands for T and L.	

[a] — ref. 11.
[b] — refs. 26—28.

The constants relating to the dispersion curve are calculated with the help of the dispersion curve measured by Kearney et al. [65]. For the simplicity of calculations, τ_B^{-1} and H are taken to be the same for transverse and longitudinal phonons in the present analysis, and are calculated at 4 and 6 K, respectively. The constants relating to the resonant phonon scattering relaxation rate τ_r^{-1} are taken from the earlier report of Dubey [16]. The point-defect scattering strength A

and the three-phonon scattering strengths B_{TN} and B_{LN} are calculated at 10 and 20 K (near the conductivity maxima), respectively, similarly as for Mg_2Si. The four-phonon scattering strengths B_{HT} and B_{HL} are also estimated similarly as for Mg_2Si, as discussed in section III. Thus, all the constants used in the calculation of the lattice thermal conductivity of Mg_2Sn are listed in Table 4, together with those for Mg_2Si.

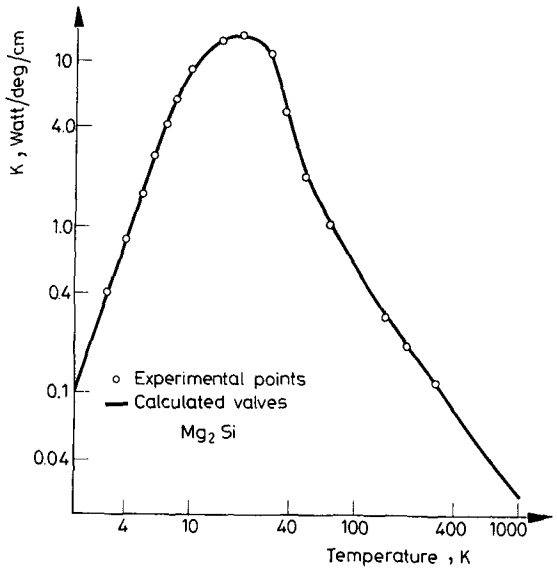

Fig. 4. The total lattice thermal conductivity of Mg_2Sn in the temperature range 2–1000 K. The solid line represents the calculated values, and circles are the experimental points

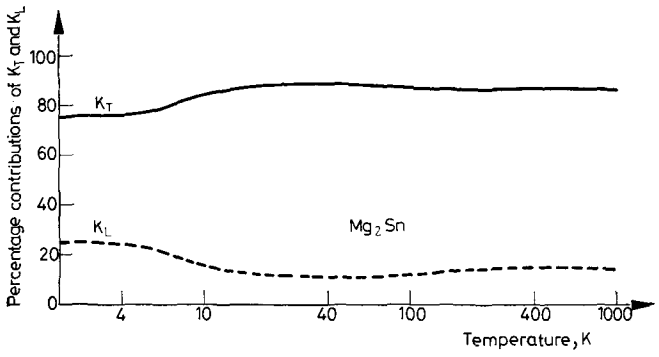

Fig. 5. The percentage contributions due to transverse and longitudinal phonons towards the total lattice thermal conductivity of Mg_2Sn. The solid line represents the percentage contribution due to transverse phonons, while the dotted line is that due to longitudinal phonons

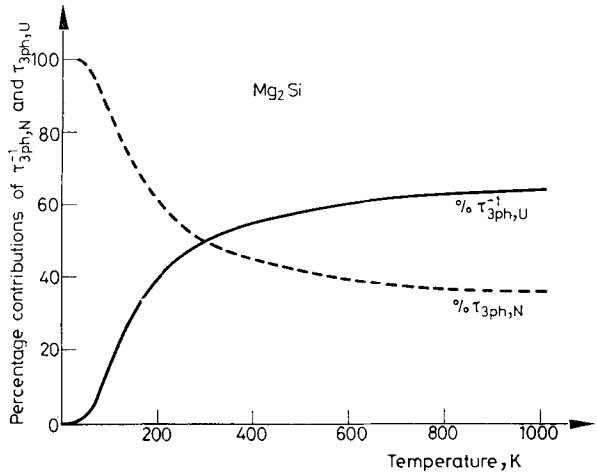

Fig. 6. The percentage contributions due to three-phonon N and U-process scattering relaxation rates towards τ_{3ph}^{-1} for Mg_2Sn. The dotted line is the percentage contribution due to the three-phonon normal process scattering relaxation rate ($\%\tau^{-1}_{3ph,N}$), and the solid line is that due to three-phonon umklapp processes

Table 8

The percentage contribution of the three-phonon scattering relaxation rate $\tau^{-1}_{3ph,T}$ towards the combined scattering relaxation rate $\tau_{c,T}^{-1}$ for transverse phonons for Mg_2Sn in the absence of four-phonon processes, for four different values of the phonon frequencies. w_{max} is the maximum frequency of transverse phonons

T K	% $\tau^{-1}_{3ph,T}$ for $w = 1/4w_{max}$	% $\tau^{-1}_{3ph,T}$ for $w = 1/2w_{max}$	% $\tau^{-1}_{3ph,T}$ for $w = 3/4w_{max}$	% $\tau^{-1}_{3ph,T}$ for $w = w_{max}$
1000	99.991	99.947	99.827	99.593
900	99.989	99.941	99.805	99.541
800	99.988	99.932	99.776	99.473
700	99.986	99.920	99.738	99.384
600	99.983	99.904	99.685	99.259
500	99.978	99.880	99.605	99.072
400	99.971	99.840	99.475	98.769
300	99.958	99.765	99.229	98.199
200	99.925	99.583	98.638	96.843
100	99.793	98.857	96.330	91.748
90	99.760	98.679	95.775	90.568
80	99.719	98.456	95.086	89.126
70	99.667	98.172	94.219	87.348
60	99.545	97.519	92.264	83.476
50	99.329	96.379	88.980	77.377
40	98.783	93.582	81.563	65.204
30	96.592	83.589	60.713	39.562
20	84.830	50.124	23.366	11.438
10	25.904	5.910	1.870	0.801
8	12.522	2.508	0.774	0.330
6	4.333	0.807	0.246	0.105
4	0.887	0.161	0.049	0.021
2	0.056	0.010	0.003	0.001

Table 9

The percentage contribution of the three-phonon scattering relaxation rate $\tau_{3ph,L}^{-1}$ towards the combined scattering relaxation rate $\tau_{c,L}^{-1}$ for longitudinal phonons for Mg_2Sn in the absence of four-phonon processes, for four different values of the phonon frequencies. w_{max} is the maximum longitudinal phonon frequency

T, K	$\% \tau_{3ph,L}^{-1}$ for $w = 1/4 w_{max}$	$\% \tau_{3ph,L}^{-1}$ for $w = 1/2 w_{max}$	$\% \tau_{3ph,L}^{-1}$ for $w = 3/4 w_{max}$	$\% \tau_{3ph,L}^{-1}$ for $w = w_{max}$
1000	99.990	99.965	99.921	99.860
900	99.989	99.960	99.911	99.842
800	99.988	99.954	99.898	99.819
700	99.985	99.947	99.880	99.788
600	99.982	99.936	99.856	99.745
500	99.978	99.919	99.820	99.680
400	99.971	99.893	99.760	99.574
300	99.957	99.842	99.647	99.375
200	99.923	99.720	99.375	98.894
100	99.789	99.230	98.293	97.008
90	99.756	99.110	98.029	96.552
80	99.714	98.959	97.699	95.984
70	99.661	98.766	97.280	95.268
60	99.537	98.322	96.319	93.643
50	99.317	97.541	94.657	90.887
40	98.761	95.601	90.660	84.530
30	97.094	90.108	80.270	69.609
20	90.817	72.945	54.630	40.401
10	55.281	25.206	13.082	7.811
8	38.761	14.716	7.155	4.158
6	21.075	6.785	3.149	1.797
4	7.332	2.111	0.954	0.539
2	0.979	0.269	0.120	0.068

From the constants reported in Table 4 and the combined scattering relaxation rates in Table 7, the total lattice thermal conductivity of Mg_2Sn has been calculated in the entire temperature range 2 – 1000 K by determining the separate contributions due to transverse and longitudinal phonons with the help of numerical integration of the conductivity integrals, similarly as for Mg_2Si, and the result obtained is shown in Fig. 4. The percentage contributions $\%K_T$ and $\%K_L$ due to transverse and longitudinal phonons, respectively, are also calculated, and the results obtained are reported in Fig. 5. The percentage contributions of $\tau_{3ph,N}^{-1}$ and $\tau_{3ph,U}^{-1}$ towards τ_{3ph}^{-1} have also been determined to examine the dominating nature of one over the other, similarly as for Mg_2Si, and the results obtained are reported in Fig. 6. The percentage contribution of τ_{3ph}^{-1} towards the combined scattering relaxation rate has been calculated for this sample too, similarly as for Mg_2Si, to inspect dominating nature of τ_{3ph}^{-1} over τ_B^{-1}, τ_{pt}^{-1} and τ_r^{-1}, and the results obtained are listed in Tables 8 and 9.

Comparative study of the present analysis with the previous studies

In this section, a comparative study of the present analysis with the previous studies has been made to consider the value of the present study. Martin and Denielson [58] analyzed the data of the lattice thermal conductivity of Mg_2Sn in the temperature range 4 – 300 K in the frame of the Callaway integral [5]. From Tables 1 and 2, it is clear that the expression they used (in the frame of the Callaway integral) for τ_{3ph}^{-1} is valid for longitudinal phonons alone. At the same time, they did not make any distinction between transverse and longitudinal phonons. They used the w^4 dependence for the resonant phonon scattering relaxation rate, which is not valid for $\hbar w \gg 4\Delta$. As a result of the above facts, they could not get good agreement between calculated and experimental values above 50 K (see Figs. 4 and 5 of ref. 58). Later, it was studied by Kumar and Verma [64] in the same temperature range, using the two-mode conduction of phonons proposed by Holland [6]. From Table 2, it is quite clear that (in the frame of Holland's model) they calculated the contribution of longitudinal phonons without considering the three-phonon U-processes in the entire range of the Brillouin zone. It is also very clear that they did not consider the three-phonon N-processes in the range $1/2\, q_{max} - q_{max}$, and three-phonon U-processes in the range $0 - 1/2\, q_{max}$, in the calculation of the lattice thermal conductivity due to transverse phonons. This means that they considered only one process (either an N or a U-process) to calculate the lattice thermal conductivity of Mg_2Sn. At the same time, they used Herring's relations [1], i.e. $\tau_{3ph,T}^{-1} \alpha T^4$ and $\tau_{3ph,L}^{-1} \alpha T^3$, in the entire temperature range, though these are valid at low temperatures only. At the same time, they could not get good agreement between calculated and experimental values of the lattice thermal conductivity of Mg_2Sn (see Fig. 1 of ref. 64).

Following Kumar and Verma, Martin [66] tried to explain his experimental data of the lattice thermal conductivities of Mg_2Sn and Mg_2Si in the temperature ranges 4 – 700 K and 4 – 300 K, respectively, by calculating the lattice thermal conductivities in the frame of the Holland model. This means that his study is similar to that of Kumar and Verma discussed above, except that he analysed up to 700 K. The lattice thermal conductivities of Mg_2Sn and MgSi were further studied by Dubey [16] in the frame of the Sharma – Dubey – Verma (SDV) model [8 – 10], in the temperature ranges 4 – 700 K and 4 – 300 K, respectively, and by Misho and Dubey [67] in the frame of the expression for τ_{ph}^{-1} proposed by Joshi and Verma [11] in the entire temperature ranges 4 – 1000 K and 3 – 500 K, respectively. From Table 2, it is clear that Dubey could not include the three-phonon N-processes and Misho and Dubey considered the contribution due to the three-phonon normal processes only, in their calculations of the lattice thermal conductivities of the above samples. However, in these analyses they were able to incorporate the Guthrie expression [7] for the temperature exponent for the three-phonon scattering relaxation rates. At the same time, a continuous temperature exponent m for the three-phonon scattering relaxation rates was used for

the first time by Dubey in the analysis of the lattice thermal conductivities of Mg_2Sn and Mg_2Si.

From Table 3 and 7, it is clear that for the first time the contributions of both N and U-processes have been included in the same conductivity integral in the analysis of the lattice thermal conductivities of Mg_2Sn and Mg_2Si at low as well as at high temperatures. The temperature exponent for the three-phonon scattering relaxation rates used in the present analysis is also free from Guthrie's comments [7, 68]. The contribution due to four-phonon processes towards the total lattice thermal resistivity is also considered at high temperatures.

Results and discussion

With the help of Figs. 1 and 4, one can see that the agreement between the calculated and experimental values of the lattice thermal conductivities of Mg_2Si and Mg_2Sn is very good in the entire temperature range 2 – 1000 K. This means that the expression $\tau_{3ph}^{-1} = (B_N + B_U e^{-\Theta/\alpha T})\, g(w)\, T^m$ proposed by Dubey and Misho gives a good response to the experimental data of the lattice thermal conductivity. From Figs. 2 and 5, it can be concluded that most of the heat is carried by the transverse phonons alone, which is similar to the findings of the previous workers. It is also similar to the result obtained in the frame of the variational technique [69 – 71]. At the same time, it is necessary to state that the nature of the variation of $\%K_T$ and $\%K_L$ is very similar to those for Si obtained by Dubey [27] in the frame of Dubey and Misho's expression for the three-phonon scattering relaxation rates. The variations of $\%\tau_{3ph,N}^{-1}$ and $\%\tau_{3ph,U}^{-1}$ with temperature can be seen in Figs. 3 and 6 for Mg_2Si and Mg_2Sn, respectively; these are very similar to those for Ge, Si, GaAs and InSb obtained by Dubey et al. [26 – 28]. From these Figures, it is clear that at low temperature $\tau_{3ph,N}^{-1}$ dominates over $\tau_{3ph,U}^{-1}$, whereas $\tau_{3ph,U}^{-1}$ dominates over $\tau_{3ph,N}^{-1}$ at high temperatures, which is in agreement with the findings of the earlier workers.

At low temperatures, the temperature exponent m tends to 4 and 3 for transverse and longitudinal phonons, respectively. At the same time, due to the large value of Θ, the exponential term $\exp(-\Theta/\alpha T)$ becomes very small at low temperatures, which results in a negligibly small contribution of the three-phonon U-processes as compared to the contribution due to the three-phonon N-processes at these temperatures. This can also be seen in Figs. 3 and 6. As a result, the expression for τ_{3ph}^{-1} used in the present analysis reduces to $\tau_{3ph,T}^{-1} = B_{TN} w T^4$ for transverse phonons, and $\tau_{3ph,L}^{-1} = B_{LN} w^2 T^3$ for longitudinal phonons. With the help of the above facts, it can be concluded that at low temperatures, the expression for τ_{3ph}^{-1} used in the present work reduces to the Herring relations, which give a good response to the low-temperature lattice thermal conductivity data.

At high temperatures, the temperature exponent m tends to unity for both modes, transverse and longitudinal phonons, and the term $\exp(-\Theta/\alpha T)$ reduces to unity due to the large value of T. Thus, the expression for τ_{3rh}^{-1} used in the present

calculations can be approximated to by $\tau_{3ph,T}^{-1} = B_T wT$ for transverse phonons, and $\tau_{3ph,L}^{-1} = B_L w^2 T$ for longitudinal phonons, which results in a T^{-1} temperature-dependence for the lattice thermal conductivity at high temperatures and is similar to the result obtained by previous workers based on theoretical as well as experimental methods.

The contribution of τ_{3ph}^{-1} towards the combined scattering relaxation rates can be studied in more detail with the help of Tables 5, 6, 8 and 9. From these Tables, it is quite clear that at high temperature, the three-phonon scattering relaxation rates dominate over boundary, point-defect and resonant phonon scattering relaxation rates. Thus, it can be concluded that at high temperatures, the lattice thermal resistivity of a sample is mainly due to the phonon-phonon scattering processes. A similar conclusion is reported by Hamilton and Parrott [69] and also by Srivastava [70, 71] based on the variational techniques. It is also similar to the results obtained by Dubey et al. [26–28] for Ge, Si, GaAs and InSb.

*

The author wishes to express his thanks to Dr. R. A. Rashid, Dr. R. H. Misho and Dr. G. S. Verma for their interest in the present work.

References

1. C. Herring, Phys. Rev., 95 (1954) 954.
2. P. G. Klemens, Solid State Physics (eds. by F. Seitz and D. Turnbull) Academic Press Inc, New York, 1958 7 (1958) 1.
3. P. G. Klemens, Proc. Roy. Soc. London, Ser. A 208 (1951) 108.
4. P. G. Klemens, Proc. Phys. Soc. London, 65 (1955) 1113.
5. J. Callaway, Phys. Rev., 113 (1959) 1046.
6. M. G. Holland, Phys. Rev., 132 (1963) 2461.
7. G. L. Guthrie, Phys. Rev., 152 (1966) 801.
8. P. C. Sharma, K. S. Dubey and G. S. Verma, Phys. Rev., B4 (1971) 1306.
9. K. S. Dubey and G. S. Verma, Phys. Rev., B4 (1971) 4491.
10. K. S. Dubey, Ph.D. Thesis (Banaras Hindu University, VARANASI-221005, India) 1971.
11. Y. P. Joshi and G. S. Verma, Phys. Rev., B1 (1970) 750.
12. R. H. Misho and K. S. Dubey, Ind. J. Pure Appl. Phys., 15 (1977) 48
13. M. D. Tiwari and B. K. Agrawal, Phys. Rev., B4 (1971) 3527.
14. M. D. Tiwari, D. N. Talwar and B. K. Agrawal, Sol. Stat. Comms., 9 (1971) 995.
15. K. S. Dubey, Phys. Rev., B13 (1976) 1836.
16. K. S. Dubey, Ind. J. Pure Appl. Phys., 12 (1974) 468.
17. K. S. Dubey, Phys. Rev., B7 (1973) 2876.
18. K. S. Dubey and G. S. Verma, Phys. Rev., B7 (1973) 2879.
19. M. G. Holland, Phys. Rev., 134 (1964) A471.
20. A. M. Toxen, Phys. Rev., 122 (1961) 450.
21. L. G. Radosevich and C. T. Walker, Phys. Rev., 171 (1968) 1004.
22. H. E. Jackson and C. T. Walker, Phys. Rev., B3 (1971) 1428.
23. R. S. Blewer, N. H. Zebouni and G. C. Grenier, Phys. Rev., 174 (1968) 700.
24. M. P. Singh and G. S. Verma, Physica, 62 (1972) 627.
25. K. C. Sood and G. S. Verma, Phys. Rev., B5 (1972) 3165.
26. K. S. Dubey and R. H. Misho, J. Thermal Anal., 15 (1978) 223.

27. K. S. DUBEY, Ind. J. Pure Appl. Phys., 15 (1977) 455.
28. M. C. AL-EDANI and K. S. DUBEY, Phys. Status Solidi, B86 (1978) 741.
29. M. C. AL-EDANI and K. S. DUBEY, Phys. Stat. Solidi B87 (1978) K47.
30. I. POMERANCHUK, Phys. Rev., 60 (1941) 82.
31. I. POMERANCHUK, J. Phys. U.S.S.R. 4 (1941) 259.
32. I. POMERANCHUK, J. Phys. U.S.S.R. 7 (1942) 197.
33. K. C. SOOD, M. P. SINGH and G. S. VERMA, Phys. Rev., B3 (1971) 385.
34. C. M. BHANDARI and G. S. VERMA, Phys. Rev., 138 (1965) A288.
35. C. M. BHANDARI and G. S. VERMA, Phys. Rev. 140 (1965) N2101.
36. K. S. DUBEY and G. S. VERMA, Phys. Rev., B5 (1972) 2215.
37. K. S. DUBEY, Ind. J. Pure Appl. Phys , 13 (1975) 302.
38. K. S. DUBEY, Phys. Status Solidi, B58 (1973) 791.
39. K. S. DUBEY, Sol. Stat. Comm., 15 (1974) 754.
40. H. H. BOGHOSSIAN and K. S. DUBEY, Phys. Status Solidi, (b)88 (1978) 417.
41. H. B. G. CASIMIR, Physica, 5 (1938) 945.
42. K. S. DUBEY, Phys. Status Solidi, B79 (1977) K119.
43. K. S. DUBEY, Phys. Status Solidi, B81 (1977) K83.
44. K. S. DUBEY, J. Physique, 47 (1976) 263
45. K. S. DUBEY, Sol. Stat. Comm., 23 (1977) 963.
46. K. S. DUBEY, Ind. J. Pure Appl. Phys., 11 (1973) 265.
47. K. S. DUBEY and G. S. VERMA, Proc. Phys. Soc. Japon, 32 (1972) 1202.
48. R. M. SAMUEL, R. H. MISHO and K. S. DUBEY, Current Sci., 46 (1977) 220.
49. Y. P. JOSHI and G. S. VERMA, Physica, 47 (1970) 213.
50. J. CALLAWAY and M. C. V. BAEVER, Phys. Rev., 120 (1960) 1149.
51. B. K. AGRAWAL and G. S. VERMA, Phys. Rev., 128 (1962) 603.
52. K. S. DUBEY, J. Phys. Chem. Solids, 39 (1978) 699.
53. V. V. KOSAREV, P. V. TAMARIN and S. S. SHALYAT, Phys. Status Solidi B44 (1971). 525.
54. J. E. PARROTT, Phys. Status Solidi, B48 (1971) K159.
55. K. S. DUBEY, Phys. Status Solidi, B63 (1974) K35.
56. P. C. SHARMA, K. S. DUBEY and G. S. VERMA, Phys. Rev., B3 (1971) 1985.
57. W. B. WHITTEN, P. L. CHUNG and G. C. DENIELSEN, J. Phys. Chem. Solids, 26 (1965) 49
58. J. J. MARTIN and G. C. DENIELSON, Phys. Rev., 166 (1968) 879.
59. P. C. KWOK, Phys. Rev., 149 (1966) 666.
60. A. GRIFFINS and P. CARRUTHERS, Phys. Rev., 131 (1963) 1976.
61. A. KUMAR, A. K. SRIVASTAVA and G. S. VERMA, Phys. Rev., B2 (1970) 4903.
62. H. H. BOGHOSSIAN and K. S. DUBEY, Phys. Status Solidi, B85 (1978) K99.
63. H. H. BOGHOSSIAN and K. S. DUBEY, Phys. Status Solidi, B89 (1978) K65.
64. A. KUMAR and G. S. VERMA, Phys. Rev., B1 (1970) 488.
65. R. J. KEARNEY, T. G. WORTTEN and R. E. SCHMUNK, J. Phys. Chem. Solids, 31 (1979) 1085.
66. J. J. MARTIN, J. Phys. Chem. Solids, 33 (1972) 1139.
67. R. H. MISHO and K. S. DUBEY, Ind. J. Phys., A52 (1977) 234.
68. G. L. GUTHRIE, Phys. Rev., B3 (1971) 3373.
69. R. A. H. HAMILTON and J. E. PAROTT, Phys. Rev., 178 (1969) 1284.
70. G. P. SRIVASTAVA, Pramana, 7 (1976) 236.
71. G. P. SRIVASTAVA, Phil. Magn. 34 (1976) 795.

RÉSUMÉ — On a étudié, dans tout l'intervalle de températures allant de 2 à 1000 K, la conductibilité thermique du réseau de Mg_2Si et Mg_2Sn, en se servant de l'expression récemment proposée par Dubey et Misho pour la vitesse de relaxation de la diffusion à trois phonons. On a trouvé un très bon accord entre les valeurs calculées et expérimentales de la conductibilité thermique du réseau dans tout l'intervalle de températures étudié. La contribution individuelle des phonons transversaux et longitudinaux, à la conductibilité thermique totale du

réseau a été étudiée de même, en calculant leurs taux respectifs de contribution. On a étudié, pour les deux échantillons, Mg_2Si et Mg_2Sn les taux respectifs de contribution dus aux processus de vitesses de relaxation de diffusion à trois phonons normaux et inversés vis-à-vis de la vitesse de relaxation de diffusion à trois phonons. On a étudié de même le pourcentage de contribution de la vitesse de relaxation de diffusion à trois phonons à la vitesse de relaxation de diffusion, résultante, pour des phonons transversaux et longitudinaux, pour quatre valeurs différentes de fréquences des phonons. Le rôle des processus à quatre phonons est aussi inclus dans la présente analyse.

ZUSAMMENFASSUNG — Die Gitter-Wärmeleitfähigkeit von Mg_2Si und Mg_2Sn wurde im ganzen Temperaturbereich von 2 bis 1000 K im Rahmen des von Dubey und Misho vorgeschlagenen Ausdrucks für die Drei-Phonon-Streuungs-Relaxationsgeschwindigkeit analysiert und eine sehr gute Übereinstimmung der berechneten und Versuchswerte der Gitter-Wärmeleitfähigkeit im ganzen untersuchten Temperaturbereich wurde gefunden. Der den transversalen und longitudinalen Phononen zuzuschreibende getrennte Beitrag zur gesamten Gitter-Wärmeleitfähigkeit wurde durch Berechnung ihres prozentualen Beitrags ebenfalls studiert. Die den Drei-Phonon-Normal- und Umklapp-Prozessen der Streuungs-Relaxationsgeschwindigkeiten zuzuschreibende prozentuale Anteil zur Drei-Phonon-Streuungs-Relaxationsgeschwindigkeit wurde für beide Proben, für Mg_2Si wie für Mg_2Sn gleichsam untersucht. Der prozentuale Beitrag der Drei-Phonon-Streuungs-Relaxationsgeschwindigkeit zur kombinierten Streuungs-Relaxationsgeschwindigkeit wurde sowohl für transversale als auch für longitudinale Phononen für vier verschiedene Werte der Phononfrequenzen ebenfalls untersucht. Die Rolle der Vier-Phonon-Prozesse wurde in die vorliegende Analyse ebenfalls aufgenommen.

Резюме — В рамках недавно предложенного Дабей и Мишо выражения для трехфононовой релаксационной скорости рассеяния исследована решеточная термическая проводимость Mg_2Si и Mg_2Sn в области температур 2—1000 К. Установлено хорошее согласие между вычисленным и экспериментальным значением решеточной термической проводимости во всей исследованной температурной области. Был также исследован процентный вклад отдельно поперечных и продольных фононов в общую решеточную термическую проводимость. Для обоих образцов исследован процентный вклад нормальных процессов рассеяния и процессов переброса в трехфононовую релаксационную скорость рассеяния. Процентный вклад трехфононовой релаксационной скорости рассеяния в комбинированную релаксационную скорость рассеяния был изучен как для продольных, так и для поперечных фононов при использовании четырех различных значений фононовых частот. В анализ включена роль четырехфононовых процессов.