Journal of Thermal Analysis, Vol. 14 (1978) 213–219

ANALYSIS OF LATTICE THERMAL CONDUCTIVITY OF GaAs AT HIGH TEMPERATURES

K. S. Dubey

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

(Received June 1, 1977)

The lattice thermal conductivity of GaAs has been analysed in the entire temperature range 100–800 K in the frame of the Sharma–Dubey–Verma (SDV) model of phonon conductivity, and very good agreement has been found between the calculated and experimental values of the lattice thermal conductivity in the entire temperature range of study. The temperature exponent $m(T)$ for the three-phonon scattering relaxation rate for GaAs has also been calculated in the above temperature range. The separate percentage contributions due to transverse and longitudinal phonons have also been studied.

It is now well established that in several semiconductors there occurs a change in the slope of the K (lattice thermal conductivity) *vs.* T (temperature) curve in the high-temperature region, and the experimental data of phonon conductivity can not be explained by one conductivity integral as given by Callaway [1]. The well-known samples are Si [2] and Ge [2]. It was Holland [2] who first introduced the two-mode conduction of phonons to explain the high-temperature data of the lattice thermal conductivities of Si and Ge. Later, the author and his co-workers [3–5] proposed a modification of the Holland model, using the Guthrie [6, 7] ideas, and this is known as the Sharma–Dubey–Verma (SDV) model [3–5] in which the phonon-phonon scattering events are classified into two groups: the class I events, in which a carrier phonon is annihilated by combination, and class II, in which the annihilation takes place by splitting.

The phonon conductivity of GaAs has been studied experimentally as well as theoretically by several workers [4, 8–10]. However, their studies are limited up to room temperature, i.e. up to 300 K only. Recently, Hunt [11] measured the thermal conductivity of GaAs in the temperature range 305–735 K. In the present work, our aim was to analyse the measurements of Hunt by calculating the lattice thermal conductivity of GaAs in the temperature range 100–800 K in the frame of the SDV model. To do so, the temperature exponent $m(T)$ for the three-phonon scattering relaxation rate was calculated in the entire temperature range 100–800 K. To study the relative contributions of each mode of the phonons, the separate percentage contributions due to transverse and to longitudinal phonons were also calculated in the entire temperature range of study and it was found that in the entire temperature range 100–800 K the percentage contribution due to longitudinal phonons. The paper is divided into four parts. The second part is devoted to a short account of the Sharma–Dubey–Verma model of lattice thermal conductivity, whereas the phonon conductivity of GaAs is dealt with in third part. The last section gives results and a discussion of the present analysis.

The Sharma–Dubey–Verma (SDV) model of lattice thermal conductivity

Recently, while commenting on the nature of dependence of the phonon conductivity on frequency w and temperature T, Guthrie [6, 7] gave an expression for the three-phonon scattering relaxation rate $\tau_{3\text{ph}}^{-1}$ in the form

$$\tau_{3\text{ph}}^{-1} \; \alpha g(w) f(T) \ldots \quad \ldots \quad \ldots \tag{1}$$

where $f(T) = T^{\text{m}}$ and $m = m(T)$. Further $g(w) = w$ for transverse phonons and $g(w) = w^2$ for longitudinal phonons. Following Klemens [12] and incorporating the Guthrie ideas, the author and his co-workers [3–5] gave an expression for $\tau_{3\text{ph}}^{-1}$ as

$$\tau_{3\text{ph}}^{-1} \; \alpha g(w) \, T^{m(T)} \, e^{-\Theta/\alpha T} \quad \ldots \quad \ldots \quad \ldots \tag{2}$$

where Θ is the Debye temperature of the sample and α is a constant which has the same meaning as given by Klemens. According to the SDV model, for transverse phonons, the expression for $\tau_{3\text{ph}}^{-1}$ reduces to

$$\tau_{3\text{ph,T}}^{-1} = B_{\text{T,I}} \quad wT^{\text{m}} \, T, I^{(\text{T})} \, e^{-\Theta/\alpha T} \quad \ldots \quad \ldots \quad \ldots \tag{3}$$

since only class I events are possible for transverse phonons. For longitudinal phonons, the above expression for the three-phonon scattering relaxation rate akes the form

$$\tau_{3\text{ph,L}}^{-1} \; = \; (B_{\text{L,I}} \, T^m \, L, \, I^{(T)} + B_{\text{L,II}} \, T^m \, L, \, II^{(T)}) \; w^2 \; e^{-\Theta/\alpha T} \ldots \tag{4}$$

The values of the temperature exponents can be expressed as

$$m_{\text{I}}(T) = x_{\text{max}}(e^x max \; - \; 1)^{-1} + 0.5x_{max} + [\ln{(1 \; + \Theta/T)}]/\ln{(T)} \quad \ldots \quad \ldots \tag{5}$$

$$m_{\text{II}}(T) = 0.5x_{\text{max}} \, e^{0.5\text{x}} \text{ max } (e^{\text{x}} \; max - 1)^{-1} + 0.5 + [\ln(1 + \Theta/T)]/\ln(T) \ldots \ldots \tag{6}$$

where $x = \hbar w_{\text{max}}/k_{\text{B}}T$.

In the above expressions the suffix T represents transverse phonons and L longitudinal phonons. Suffixes I and II refer to class I and class II events, respectively. The B's are the corresponding scattering strengths.

In the SDV model, a better dispersion relation [13], $q = [w/v]\,(1 + rw^2)$, is used to calculate phase and group velocities inside the conductivity integral, which gives phase velocity $v_{\text{p}} = v/(1 + rw^2)$ and group velocity $v_{\text{g}} = v/(1 + 3rw^2)$, where r is a constant and can be calculated with the help of the dispersion curve as [13]

$$r = w^{-2}\,(qv/w - 1) \quad \ldots \quad \ldots \quad \ldots \tag{7}$$

Thus, using the above expressions for the three-phonon scattering relaxation rate $\tau_{3\mathrm{ph}}^{-1}$ and the correction factor due to the dispersion of phonons, the expression for the lattice thermal conductivity in the frame of the SDV model can be expressed as

$$K = K_T + K_L \quad \dots \quad \dots \quad \dots \tag{8}$$

where K_T and K_L are the phonon conductivities due to transverse and longitudinal phonons, respectively, and can be expressed as

$$\begin{aligned} K_T = {} & (C/v_{\mathrm{T1}}) \int_0^{\Theta_1/T} x^4 e^x (e^x - 1)^{-2} (1 + R_1 x^2 T^2)^2 (1 + 3R_1 x^2 T^2)^{-1} \tau_{\mathrm{c,T}} \,\mathrm{d}x + \\ & + (C/v_{\mathrm{T2}}) \int_{\Theta/T}^{\Theta_2/T} x^4 e^x (e^x - 1)^{-2} (1 + R_2 x^2 T^2)^2 (1 + 3R_2 x^2 T^2)^{-1} \tau_{\mathrm{c,T}} \,\mathrm{d}x \\ & \dots\dots\dots \end{aligned} \tag{9}$$

$$\begin{aligned} K_L = {} & (C/2v_{\mathrm{L1}}) \int_0^{\Theta/{}_4T} x^4 e^x (e^x - 1)^{-2} (1 + R_4 x^2 T^2)^2 (1 + 3R_4 x^2 T^2)^{-1} \tau_{\mathrm{c,L}} \,\mathrm{d}x + \\ & + (C/2v_{\mathrm{L2}}) \int_{\Theta_4/T}^{\Theta_3/T} x^4 e^x (e^x - 1)^{-2} (1 + R_3 x^2 T^2)^2 (1 + 3R_3 x^2 T^2)^{-1} \tau_{\mathrm{c,L}} \,\mathrm{d}x \\ & \dots \quad \dots \quad \dots \end{aligned} \tag{10}$$

where $C = (k_{\mathrm{B}}/3\pi^2)(k_{\mathrm{B}}T/\hbar)^3$, $R_{\mathrm{i}} = r_{\mathrm{i}}(k_{\mathrm{B}}/\hbar)^2$, k_{B} is the Boltzmann constant, $\hbar$ is the Planck constant divided by 2π, the v's are the velocities of corresponding modes, the Θ's are the temperatures corresponding to the Brillouin Zone boundary (for details see refs [3]–[5]), $\tau_{\mathrm{c,T}}$ and $\tau_{\mathrm{c},L}$ are the combined scattering relaxation times due to transverse and longitudinal phonons, respectively; these terms can be expressed as

$$\tau_{c,T}^{-1} = \tau_B^{-1} + \tau_{pt}^{-1} + \tau_{3\mathrm{ph},T}^{-1} \quad \text{and} \quad \tau_{c,L}^{-1} = \tau_B^{-1} + \tau_{pt}^{-1} + \tau_{3ph,L}^{-1}$$

where τ_B^{-1} and τ_{pt}^{-1} are the scattering relaxation rates due to boundary scattering and point defect scattering, respectively, according to Casimir [14] and Klemens [12, 15, 16]. These scattering relaxation rates can be expressed as $\tau_B^{-1} = v/L$ and $\tau_{pt}^{-1} = Aw^4$, where L is the Casimir length [14] of the sample under study and A is the point defect scattering [12, 15, 16] strength.

Analysis of lattice thermal conductivity of GaAs

Recently, Hunt [11] measured the thermal conductivity of GaAs in the temperature range 305–735 K. With the help of the Lorenz number and his measurements of the electrical conductivity of the same sample, the lattice part of the thermal conductivity, i.e. the lattice thermal conductivity of GaAs, was separated by subtracting the electronic part of the thermal conductivity from the total thermal conductivity measured by Hunt. Thus, the experimental data for the analysis of the lattice thermal conductivity were taken from the earlier report of Holland (in the temperature range 100–300 K) and Hunt (305–735 K). The constants relating to the dispersion curve were calculated from the experimental dispersion curve of GaAs reported by Waugh and Dolling [17]. As stated earlier, the present study was limited to high temperatures (i.e. 100–800 K); the boundary scattering relaxation rate was ignored in the present analysis due to its negligibly small contribution to the combined scattering relaxation rate at high temperatures. The point defect scattering strength A depends on the crystal impurities (point defects). The samples used for the measurements of thermal conductivity by Holland and Hunt were different from each other, which suggests that one should assign different values of A in the temperature range 100–300 K (for the measurement of Holland) and in the temperature range 305–800 K (for the measurement of Hunt). However, it was found that for a normal sample (undoped) the high-temperature data of phonon conductivity are not very sensitive to the point defect scattering strength A. At the same time, it was also found that the measurements of Holland (K *vs.* T curve in the temperature range 100–300 K) and Hunt (K *vs.* T curve in the temperature range 305–735 K) join very smoothly to each other in the temperature range 300–305 K, which tells us that the value of A is approximately the same for the two samples. Keeping in view the above facts, the point defect scattering strength A was taken as the same for both of the measurements in the present analysis, and it is the same as reported by Dubey and Verma [4] for GaAs based on the experimental data reported by Holland.

Following the earlier work of the author [18–20] the three-phonon scattering strengths $B_{T,\mathrm{I}}$, and $B_{L,\mathrm{I}}$ and $B_{L,\mathrm{II}}$ were adjusted at 700 K, and it was found that the term $B_{L,\mathrm{I}}$ can be ignored due to its very small contribution; this is similar to the previous findings of Dubey and Verma [21]. The constants and the parameters used in the present analysis of the phonon conductivity of GaAs are listed in Table 1. Using the constants reported in this Table, the temperature exponent $m(T)$ was calculated for both transverse and longitudinal phonons in the entire

Table 1

The constants and parameters used in analysis of the lattice thermal conductivity of GaAs in the temperature range 100–800 K

$v_{T1} = 2.48 \cdot 10^{5}$ cm/sec
$v_{T2} = 0.90 \cdot 10^{5}$ cm/sec
$\Theta_1 = 90$ K
$\Theta_2 = 101.5$ K
$\Theta = 345$ K
$r_1 = 2.084 \cdot 10^{-27}\ \mathrm{sec}^2$
$r_2 = 7.225 \cdot 10^{-27}\ \mathrm{sec}^2$
$B_{T,I} = 2.04 \cdot 10^{-6}\ \mathrm{deg}^{-m}$
$A = 1.30 \cdot 10^{-44}\ \mathrm{sec}^3$

$v_{L1} = 4.73 \cdot 10^{5}$ cm/sec
$v_{L2} = 4.73 \cdot 10^{5}$ cm/sec
$\Theta_4 = 187$ K
$\Theta_3 = 313$ K
$\alpha = 2.0$
$r_4 = 0$
$r_3 = 1.163 \cdot 10^{-28}\ \mathrm{sec}^2$
$B_{L,II} = 2.07 \cdot 10^{-18}\ \mathrm{sec\ deg}^{-m}$

Table 2

The value of temperature exponent $m(T)$ obtained using Eqs (5) and (6), used to calculate the lattice thermal conductivity of GaAs. $m_{T,I}(T)$ is the temperature exponent of the three-phonon scattering relaxation rate due to transverse phonons for class I events, whereas $m_{L,I}(T)$ and $m_{L,II}(T)$ are the same for longitudinal phonons for class I and class II events, respectively

T, K	$m_{T,I}(T)$	$m_{L,I}(T)$s	$m_{L,II}(T)$
100	1.3021	1.4934	1.0
200	1.1388	1.1892	1.0
300	1.0892	1.1118	1.0
400	1.0652	1.0780	1.0
500	1.0511	1.0593	1.0
600	1.0419	1.0476	1.0
700	1.0354	1.0396	1.0
800	1.0306	1.0338	1.0

temperature range 100 – 800 K with the help of Eqs (5) and (6) and the obtained results are reported in Table 2. Using the constants and parameters listed in Table 1 and the temperature exponents $m(T)$ for the three-phonon scattering relaxation rates reported in Table 2, the lattice thermal conductivity of GaAs was calculated by calculating the separate contributions due to transverse and longitudinal phonons. The results is shown in Fig. 1. The entire calculations were performed by numerical integration of the conductivity integrals reported in Eqs (9) and (10). To study the relative contributions due to transverse and longitudinal phonons, the separate percentage contributions due to each mode of the

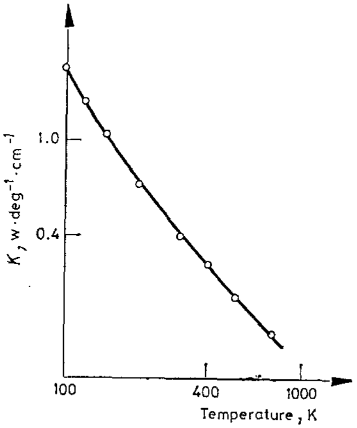

Fig. 1. The lattice thermal conductivity of GaAs in the temperature range 100—800 K. The solid line shows the calculated values and the circles are the experimental points

Table 3

The relative contributions of transverse and longitudinal phonons for GaAs in the temperature range 100—800 K. $\%K_T$ is the percentage contribution of transverse phonons and $\%K_L$ that of longitudinal phonons

T, K	%, K_T	%, K_L
100	77.68	22.32
200	85.11	14.89
300	87.46	12.54
400	88.61	11.39
500	89.30	10.70
600	89.72	10.28
700	90.07	9.93
800	90.31	9.69

phonons were also calculated in the entire temperature range of study, and the results are listed in Table 3.

Results and discussions

From Fig. 1, the agreement between the calculated and experimental values of the phonon conductivity of GaAs can be seen to be very good in the entire temperature range 100–800 K, and the high-temperature data on the phonon conductivity of GaAs can be explained in the frame of the SDV model of lattice thermal conductivity. From Table 3, it is very clear that the percentage contribution due to transverse phonons is much larger than that due to longitudinal phonons in the entire temperature range 100–800 K. At the same time, it can also be concluded that the relative contribution of transverse phonons (i.e. $\%K_T$) increases with increase of temperature. Thus, one can say that at high temperatures almost all the heat is carried by transverse phonons alone. This result is similar to the previous findings of several workers [22–26] in the frame of the relaxation time approach. At the same time, it is also similar to the earlier findings of Hamilton and Parrott [27] based on the variational method. From Table 2, it can be seen that the temperature exponent $m(T)$ for the three-phonon scattering relaxation rates used in the present analysis is free from the Guthrie comments about it. Thus, for the first time, the lattice thermal conductivity of GaAs has been analysed at high temperature (above 300 K) using a suitable value of the temperature exponent $m(T)$ for the three-phonon scattering relaxation rate which is free from the Guthrie comments, and a very good agreement has been achieved between the calculated and experimental values of the phonon conductivity.

*

The author wishes to express his thanks to Dr. R. A. Rashid and Dr. G. S. Verma for their constant encouragement. He is also grateful to Dr. R. H. Misho for supplying the necessary and useful data.

References

1. J. CALLAWAY, Phys. Rev., 113 (1959) 1046.
2. M. G. HOLLAND, Phys. Rev., 132 (1963) 2461.
3. P. C. SHARMA, K. S. DUBEY and G. S. VERMA, Phys. Rev., Ser. B., 4 (1971) 1306.
4. K. S. DUBEY and G. S. VERMA, Phys. Rev., Ser. B., 4 (1971) 4491.
5. K. S. DUBEY, Ph. D. Thesis (Banaras Hindu University, Varanasi 221005, India) 1971.
6. G. L. GUTHRIE, Phys. Rev., 152 (1966) 801.
7. G. L. GUTHRIE, Phys. Rev., Ser. B., 3 (1971) 3373.
8. M. G. HOLLAND, Phys. Rev., 134 (1964) 471.
9. C. M. BHANDARI and G. S. VERMA, Phys. Rev., 140 (1965) 2101.
10. M. D. TIWARI, D. N. TALWAR and B. K. AGRAWAL, Sol. Stat. Comms., 9 (1971) 995.
11. D. R. HUNT, Ph. D. Thesis (University Coll. Swansea, U. K.) 1974.
12. P. G. KLEMENS, Solid State Phys., 7 (1958) 1.
13. P. C. SHARMA, K. S. DUBEY and G. S. VERMA, Phys. Rev., Ser. B., 3 (1971) 1985.
14. H. B. G. CASIMIR, Physica, 5 (1938) 945.
15. P. G. KLEMENS, Proc. Phys. Soc., London, Ser. A., 68 (1955) 1113.
16. P. G. KLEMENS, Proc. Phys. Soc., London, Ser. A., 70 (1957) 833.
17. J. L. T. WAUGH and G. DOLLING, Phys. Rev., 132 (1963) 2410.
18. K. S. DUBEY, Ind. J. Pure Appl. Phys., 12 (1974) 468.
19. K. S. DUBEY, Phys. Rev., Ser. B., 7 (1973) 2876.
20. K. S. DUBEY, Phys. Rev., Ser. B., 13 (1976) 1836.
21. K. S. DUBEY and G. S. VERMA, Phys. Rev., Ser. B., 7 (1973) 2879.
22. R. H. MISHO and K. S. DUBEY, Ind. J. Pure Appl. Phys., 15 (1977) 48.
23. M. D. TIWARI and B. K. AGRAWAL, Phys. Rev., Ser. B., 4 (1971) 3527.
24. A. KUMAR and G. S. VERMA, Phys. Rev., Ser. B., 1 (1970) 488.
25. Y. P. JOSHI and G. S. VERMA, Phys. Rev., Ser. B., 1 (1970) 750.
26. R. H. MISHO and K. S. DUBEY, Ind. J. Phys., (1978 in press)
27. R. A. H. HAMILTON and J. E. PARROTT, Phys. Rev., 178 (1969) 1284.

RÉSUMÉ — La conductibilité thermique du réseau de GaAs a été analysée dans tout l'intervalle de température allant de 100 à 800 K, dans le cadre du modèle de conductibilité de phonons de Sharma—Dubey—Verma (SDV). Une très bonne concordance a été observée entre les valeurs calculées et expérimentales de la conductibilité thermique du réseau dans l'intervalle de température étudié. L'exposant de température $m(T)$ a également été calculé dans ce domaine de température pour la vitesse de relaxation de la diffusion de trois phonons. Les pourcentages individuels des contributions des phonons transversaux et longitudinaux ont également été étudiés.

ZUSAMMENFASSUNG — Die Gitter-Warmeleitfähigkeit von GaAs wurde im Temperaturbereich zwischen 100 und 800 K im Rahmen des Modells der Phononen-Leitfähigkeit von Sharma—Dubey—Verma (SDV) untersucht und eine sehr gute Übereinstimmung zwischen den berechneten und Versuchswerten der Gitter-Wärmeleitfähigkeit im ganzen untersuchten Temperaturbereich gefunden. Der Temperaturexponent $m = m(T)$ für die Drei-Phonenen-Streuungs-Relaxationsgeschwindigkeit bei GaAs wurde im obengenannten Temperaturbereich ebenfalls berechnet. Die durch transversale und longitudinale Phonone verursachten einzelnen prozentualen Beiträge wurden ebenfalls untersucht.

Резюме — В области температур 100—800 К была проанализирована решеточная термическая проводимость CaAs на основе Шарма-Дьюби-Верма модели фононовой проводимости. Найдено очень хорошее согласие между вычисленными и экспериментальными значениями решеточной термической проводимости во всей изученной области температур. Вычислена температурная экспонента $m(T)$ релаксационной скорости трехфононового рассеивания для CaAs. Были также изучены отдельные вклады, обусловленные продольными и поперечными фононами.