Acta Physica Hungarica, 63 (3—4), pp. 331–340 (1988)

PHONON CONDUCTIVITY OF InSb IN THE TEMPERATURE RANGE 2–800 K

A. H. AWAD

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

(Received in revised form 12 May 1986)

The lattice thermal conductivity of InSb has been calculated in the temperature range 2–800 K in the frame of Dubey's model, which makes use of Guthrie's classification of three-phonon scattering events. Excellent agreement has been found between the theoretical and experimental values of the phonon conductivity over a wide range of temperatures. The temperature dependence of three-phonon scattering relaxation rate has been calculated for both class I and class II events in the study of phonon conductivity of InSb. The percentage contributions of transverse and longitudinal phonons have been studied separately in the temperature range of investigation. The role of four-phonon processes is also included at high temperatures. The percentage contributions of the three-phonon normal and umklapp processes towards τ_{3ph}^{-1} have also been investigated.

1. Introduction

The lattice thermal conductivity of InSb has been studied by several workers [1–5] experimentally as well as theoretically at low and high temperatures, and it is now established that the Callaway [6] model could not get good agreement in the high temperature region. It should be noted that the Callaway model is an exception due to the fact that it does not make any distinction between transverse and longitudinal phonons. Holland [1] modified the Callaway model, making it applicable at all temperatures by considering the two mode conduction of phonons.

The three phonon scattering relaxation rates were further studied by Guthrie [7] by dividing the phonon–phonon scattering events into two classes: Class I events in which the carrier phonon is annihilated by combination, and class II events in which annihilation takes place by splitting. Recently, considering the rate of $\tau_{3ph,N}^{-1}$ and $\tau_{3ph,U}^{-1}$ and following Guthrie's classification of the phonon–phonon scattering events Dubey [8] studied the thermal conductivity of a sample by proposing a new expression for τ_{3ph}^{-1} as

$$\tau_{3ph}^{-1}=(B_{N,\mathrm{I}}+B_{U,\mathrm{I}}e^{-\theta/\alpha T})g(w)T^{m_{\mathrm{I}}(T)}+ \\ +(B_{N,\mathrm{II}}+B_{U,\mathrm{II}}e^{-\theta/\alpha T})g(w)T^{m_{\mathrm{II}}(T)}. \tag{1}$$

Terms are explained in the following Section. The aim of the present work is to calculate the lattice thermal conductivity of InSb in the frame of the expression for the three-phonon scattering relaxation rate proposed by Dubey. The separate contribution of transverse and longitudinal phonons towards the total lattice thermal conductivity has also been studied by calculating their percentage contributions. The percentage contribution of the three N and U processes scattering relaxation rates toward τ_{3ph}^{-1} have been studied.

2. Theory

In the present model Dubey [8] used the same frequency dependence $g(w)$ for N and U-processes due to the fact that $g(w)$ depend only on polarisation branches. At the same time, the same value of $m(T)$ is used to both N and U-processes due to the fact that Guthrie [7] obtained the same value of $m(T)$ for both processes. The temperature exponent $m(T)$ has four values 1, 2, 3 and 4 for transverse phonons and three values 1, 2 and 3 for the longitudinal phonons corresponding to the different temperature ranges. Due to lack of an expression for the exact value of $m(T)$, Dubey [8] suggested the use of the average value of the upper and lower bounds of $m(T)$ reported by Guthrie [7]. Thus, the expression for $m(T)$ used in the present communication is given by

$$m_{\mathrm{I}}(T)=X_{\max}(e^{X_{\max}}-1)^{-1}+0.5X_{\max} \tag{2}$$

for class I events and

$$m_{\mathrm{II}}(T)=0.5+0.5X_{\max}e^{0.5X_{\max}}(e^{X_{\max}}-1)^{-1} \tag{3}$$

for class II events, where $X_{\max}=\hbar w_{\max}/K_B T$, $\hbar$ is the Planck constant divided by 2π, K_B is the Boltzmann constant and $w_{\max}$ is the phonon frequency at the boundary of the Brillouin zone.

The Guthrie [7] classification leads to the participation of transverse phonons in class I events only, while longitudinal phonons participate in class I as well as in class II. As a result, Dubey [8] proposed an expression for $\tau_{3ph,T}^{-1}$ for transverse phonons as

$$\tau_{3ph,T}^{-1}=(B_{TN,\mathrm{I}}+B_{TU,\mathrm{I}}e^{-\theta/\alpha T})wT^{m_{T,\mathrm{I}}(T)}. \tag{4}$$

Similarly, the expression for $\tau_{3ph,L}^{-1}$ for longitudinal phonons is given by

$$\begin{aligned}\tau_{3ph,L}^{-1}=&(B_{LN,\mathrm{I}}+B_{LU,\mathrm{I}}e^{-\theta/\alpha T})w^2T^{m_{L,\mathrm{I}}(T)};\\ &+(B_{LN,\mathrm{II}}+B_{LU,\mathrm{II}}e^{-\theta/\alpha T})w^2T^{m_{L,\mathrm{II}}(T)},\end{aligned} \tag{5}$$

where B_N and B_U are the scattering strength of three-phonon normal and umklapp processes, respectively, suffixes N and U are used to represent normal and umklapp

processes, θ is the Debye temperature of the sample and α is a constant, $g(w)$ is the function of phonon frequency w, $g(w)=w^2$ for longitudinal phonons and w for transverse phonons which are the same as obtained by Herring [9].

The phase and group velocities of phonons inside the conductivity integral have been corrected by using a modified dispersion relation [4, 10]

$$k=(w/v)(1+rw^2), \tag{6}$$

where k is the phonon wave vector, w is the phonon frequency, r is a constant which depends on the dispersion curve of the sample under study and can be calculated with the help of the experimental dispersion curve and v is the phonon velocity.

Assuming spherical symmetry of Brillouin zone for all three polarization branches, one longitudinal and two transverse, and that each phonon contributes separately towards the total lattice thermal conductivity, the contribution of each branch can be expressed as [6]

$$K_i=(1/6\pi^2)\int \tau_{ci}V_{gi}^2(\hbar^2w^2/K_BT^2)(e^{\hbar w/K_BT}-1)^{-2} e^{\hbar w/K_BT}k^2dk+\Delta K, \tag{7}$$

where the integral is performed over the first Brillouin zone, suffix i stands for polarization branches. Vg is the group velocity corresponding to the polarization branch, ΔK is the correction term [6] due to the three phonon N-processes and its contribution can be ignored [11–13] compared to the contribution due to the first term in Eq. (7) and τ_{ci}^{-1} is the combined scattering relaxation rate given by

$$\tau_c^{-1}=\tau_B^{-1}+\tau_{pt}^{-1}+\tau_{3ph}^{-1}+\tau_{4ph}^{-1}, \tag{8}$$

where τ_B^{-1} is the boundary scattering relaxation rate [14], τ_{pt}^{-1} is the point defect scattering relaxation rate [15], τ_{3ph}^{-1} is the three-phonon scattering relaxation rate [8] and τ_{4ph}^{-1} is the four-phonon scattering relaxation rate [16, 17]. The expressions used for the scattering relaxation rates are given in Table I. The expression for the lattice thermal conductivity in the frame of SDV [10] model 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, and are given by

$$K_T=\left(\frac{c}{v_{T1}}\right)\int_0^{\theta_1/T}\tau_{c,T}x^4e^x(e^x-1)^{-2}(1+R_1x^2)^2(1+3R_1x^2)^{-1}dx+ +\left(\frac{c}{v_{T2}}\right)\int_{\theta_1/T}^{\theta_2/T}\tau_{c,T}x^4e^x(e^x-1)^{-2}(1+R_2x^2)^2(1+3R_2x^2)^{-1}dx, \tag{10}$$

$$K_L = \left(\frac{c}{2v_{L1}}\right) \int_0^{\theta_3/T} \tau_{c,L} x^4 e^x (e^x - 1)^{-2} (1 + R_3 x^2)^2 (1 + 3R_3 x^2)^{-1} dx +$$

$$+ \left(\frac{c}{2v_{L2}}\right) \int_{\theta_3/T}^{\theta_4/T} \tau_{c,L} x^4 e^x (e^x - 1)^{-2} (1 + R_4 x^2)^2 (1 + 3R_4 x^2)^{-1} dx, \qquad (11)$$

where

$$c = \frac{K_B}{3\pi^2}\left(\frac{K_B T}{\hbar}\right)^3, \quad R_i = r_i (K_B T/\hbar)^2, \quad \theta_i = \hbar w_i / K_B,$$

$i = 1, 2, 3$ and 4, r_1 and r_2 are dispersion constants for transverse phonons in the ranges $0 - 1/2k_{\max}$ and $1/2k_{\max} - k_{\max}$, respectively, r_3 and r_4 are the same for longitudinal phonons, v_{T1} and v_{T2} are the transverse phonon velocities in the range

Table I

Scattering relaxation rates. In these expressions v is the average phonon velocity, L is the Casimir length of the crystal, A is the point defect scattering strength, V is the atomic volume, f_i is the atomic fraction of the i-th impurity whose mass is m_i, m is the mass of the host lattice, $\Delta m = m - m_i$, B's are constant and $k_{\max}$ is the zone boundary of the first Brillonin zone

Scattering processes	Relaxation rates
Crystal boundary [14]	$\tau_B^{-1} = v/L$
Impurities [15]	$\tau_{pt}^{-1} = Aw^4, \quad A = \frac{V}{4\pi v_{si}^3} f_i \left(\frac{\Delta m}{m}\right)^2$
Three-phonon processes	τ_{3ph}^{-1}
Normal processes [9] (N-processes)	$\tau_{3ph,N}^{-1}$
Transverse	$\tau_{TN}^{-1} = B_T w T^4$ at low temperatures
Longitudinal	$\tau_{LN}^{-1} = B_L w^2 T^3$
Transverse	$\tau_{TN}^{-1} = B'_T w T$ at high temperature
Longitudinal	$\tau_{LN}^{-1} = B'_L w^2 T$
Umklapp processes (U processes)	$\tau_{3ph,U}^{-1}$
Klemens [25]	$\tau_U^{-1} = B_U w^2 T^3 e^{-\vartheta/\alpha T}$ at low temperature
Klemens [26]	$\tau_U^{-1} = B'_U w T^3 e^{-\vartheta/\alpha T}$
Holland [1] (for transverse)	$\tau_U^{-1} = B_{TU} w^2 / \sinh(\hbar w/K_B T)$ $1/2k_{\max} - k_{\max}$
	$\tau_U^{-1} = 0, \qquad 0 - k_{\max}$
Callaway [6]	$\tau_U^{-1} = B_U w^2 T^3$
Klemens [26]	$\tau_U^{-1} = B'_U w^2 T$ at high temperature
Four-phonon processes [16, 17]	$\tau_{4ph}^{-1} = B w^2 T^2$

$0-1/2k_{max}$ and $1/2k_{max}-k_{max}$. v_{L1} and v_{L2} are the same for longitudinal phonons, w_1 and w_3 are the frequencies of transverse and longitudinal phonons at $1/2k_{max}$, respectively, and w_2 and w_4 are the same at k_{max}.

3. Results and discussion

The boundary scattering relaxation rates $\tau_{B,T}^{-1}$, $\tau_{B,L}^{-1}$ and the point-defect scattering strength A have been adjusted at 2 K and 8 K, respectively. At low temperatures, $\tau_{3ph,N}^{-1} \gg \tau_{3ph,U}^{-1}$. Thus an approximate value of $B_{TN,I}$, $B_{LN,I}$ and $B_{LN,II}$ have been calculated at 15 K ignoring the contribution due to $\tau_{3ph,U}^{-1}$. The three-phonon U-processes dominate over N-processes at high temperatures. Therefore, one can neglect the role of three-phonon N-processes. $B_{TU,I}$, $B_{LU,I}$ and $B_{LU,II}$ at 200 K have been estimated. The four-phonon scattering strength B_{HT} and B_{HL} are calculated at 600 K. The experimental data are taken from the earlier report of Holland [18] and other constants related to the dispersion curve are taken from the earlier report of Dubey et al [4].

Using the constants and parameters reported in Table II, the lattice thermal conductivity of InSb has been calculated in the temperature range 2–800 K in the frame of the expression proposed by Dubey [8] by calculating the contribution of the transverse and longitudinal phonons separately. The results shown in Fig. 1 are in good agreement with the experimental data, also near conductivity maxima in which region Dubey and Verman [4] did not observe good agreement. The separate

Table II

Values of constants and parameters used in the calculation of phonon conductivity of InSb in the temperature range 2–800 K

v_{T1} (cm/s)	2.28×10^5	$B_{TN,I}$(deg^{-m})	1.0×10^{-12}
V_{T2} (cm/s)	0.82×10^5	$B_{TU,I}$(deg^{-m})	4.25×10^{-6}
v_{L1} (cm/s)	3.77×10^5	$B_{LN,I}$(s · deg^{-m})	1.0×10^{-23}
v_{L2} (cm/s)	3.77×10^5	$B_{LU,I}$(s · deg^{-m})	1.0×10^{-20}
O_1 (K)	56	$B_{LN,II}$(s · deg^{-m})	1.0×10^{-21}
O_2 (K)	62	$B_{LU,II}$(s · deg^{-m})	2.0×10^{-17}
O_3 (K)	101.5	B_{HT}(s · deg^{-2})	1.0×10^{-24}
O_4 (K)	170	B_{HL}(s · deg^{-2})	1.0×10^{-23}
O_D (K)	172.5		
α	1.5		
r_1 (s^2)	9.665×10^{-27}		
r_2 (s^2)	2.618×10^{-27}		
r_3 (s^2)	0		
r_4 (s^2)	1.37×10^{-27}		
τ_{BT}^{-1} (s^{-1})	4×10^5		
τ_{BL}^{-1} s^{-1})	4.2×10^5		
A (s^3)	4.2×10^{-44}		

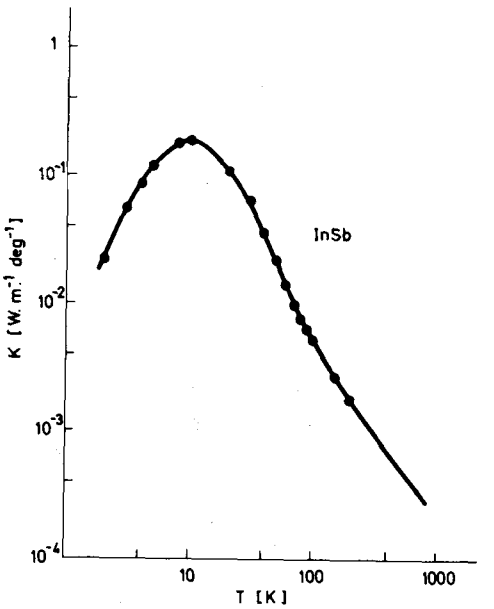

Fig. 1. Total lattice thermal conductivity of InSb in the temperature range 2–800 K. Solid line shows the calculated values and circles are the experimental points

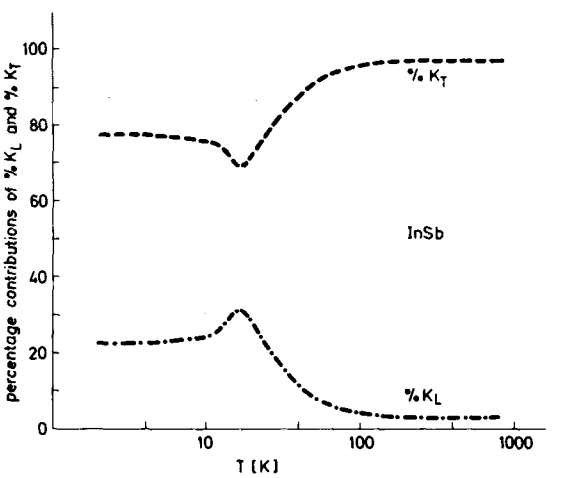

Fig. 2. The percentage contributions $\%\, K_T$ and $\%\, K_L$ towards the total lattice thermal conductivity of InSb due to transverse and longitudinal phonons, respectively. Dashed and dot–dash lines represent $\%\, K_T$ and $\%\, K_L$, respectively

percentage contributions of transverse and longitudinal phonons towards the total lattice thermal conductivity can be studied with the help of Fig. 2. From Fig. 2 it can be seen that at high temperatures the transverse phonons are mainly responsible for the transfer of heat, which is in agreement with the results reported by previous workers [1, 5, 19–23]. It is also clear that in the low temperature region the ratio $\% K_T/\% K_L$ depends upon the factor

$$2(v_L\tau_{B,L}^{-1}/v_T\tau_{B,T}^{-1}) = 2(v_L/v_T)^2$$

which indicates that at very low temperature $\% K_T$ is larger than $\% K_L$. At higher temperature towards the conductivity maxima, $\% K_T$ begins to decrease while the reverse is true for longitudinal phonons. At a certain temperature, the transverse contribution begins to increase again. This nature of such variation in the curve is due to the role of the point-defect scattering [10]. A similar nature is also obtained by Sharma et al. [10] for Ge, Dubey and Verma [24] for Si, Awad and Dubey [23] for Mg_2Ge and Mg_2Si and Al-Edani et al [5] for InSb and GaAs.

Table III

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

T[K]	$m_{T,I}(T)$	$m_{L,I}(T)$	$m_{L,II}(T)$
2	4	3	0.5
4	4	3	0.5
6	4	3	0.5
8	3.8783	3	0.5002
10	3.1120	3	0.5017
20	1.6962	3	0.5606
30	1.3329	2.8530	0.6672
40	1.1926	2.1865	0.7579
50	1.1249	1.8173	0.8212
60	1.0874	1.5937	0.8650
70	1.0645	1.4490	0.8954
80	1.0495	1.3507	0.9169
90	1.0392	1.2810	0.9327
100	1.0318	1.2299	0.9445
200	1.0079	1.0594	0.9852
300	1.0035	1.0266	0.9933
400	1.0020	1.0150	0.9962
500	1.0012	1.0096	0.9975
600	1.0008	1.0066	0.9983
700	1.0006	1.0049	0.9987
800	1.0005	1.0037	0.9990

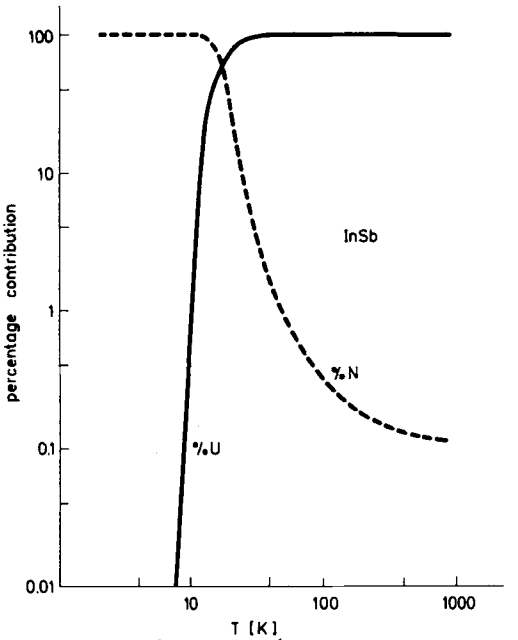

Fig. 3. The percentage contributions $\%\,\tau^{-1}_{3ph,N}$ and $\%\,\tau^{-1}_{3ph,U}$ processes towards the $\tau^{-1}_{3ph,T}$ for class I events for transverse phonons for InSb in the temperature range 2–800 K. Solid and dashed lines represent $\%\,\tau^{-1}_{3ph,U}$ and $\%\,\tau^{-1}_{3ph,N}$, respectively

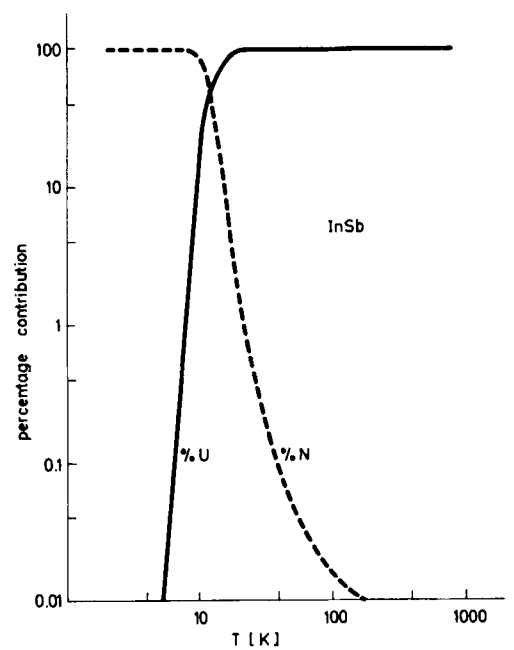

Fig. 4. The percentage contributions $\%\,\tau^{-1}_{3ph,N}$ and $\%\,\tau^{-1}_{3ph,U}$ processes towards $\tau^{-1}_{3ph,L}$ for class I events for longitudinal phonons for InSb in the temperatures range 2–800 K. Solid and dashed lines represent $\%\,\tau^{-1}_{3ph,U}$ and $\%\,\tau^{-1}_{3ph,N}$, respectively

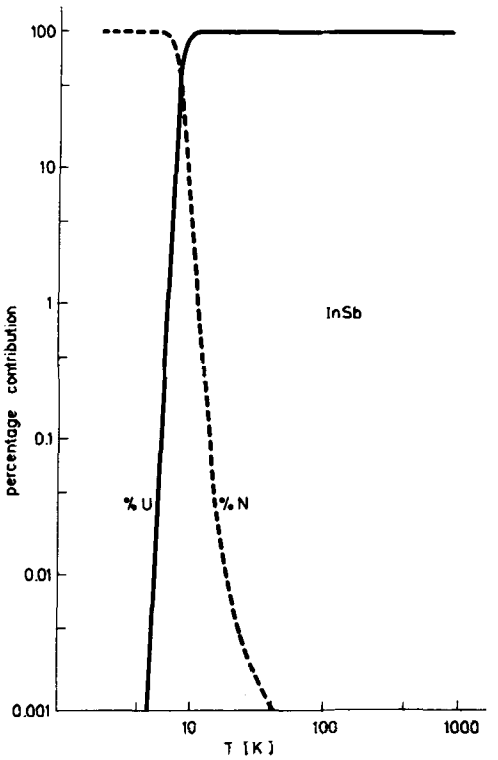

Fig. 5. The percentage contributions $\%\ \tau_{3ph,N}^{-1}$ and $\%\ \tau_{3ph,U}^{-1}$ towards $\tau_{3ph,L}^{-1}$ for class II events for InSb in the temperature range 2–800 K. Solid and dashed lines represent $\%\ \tau_{3ph,U}^{-1}$ and $\%\ \tau_{3ph,N}^{-1}$, respectively

The temperature exponents can be calculated for both transverse and longitudinal phonons in the temperature range of study with the help of Eqs (2) and (3) and the results obtained are reported in Table III. It can be seen that at low temperatures $m_{T,I}(T)$ and $m_{L,I}(T)$ tend to 4 and 3, respectively, which is similar to the results obtained by Herring [9]. It can be seen that at high temperatures $m_{T,II}(T)$, $m_{L,II}(T)$ and $m_{L,III}(T)$ tend to unity. Thus τ_{3ph}^{-1} reduces to $\tau_{3ph}^{-1} \propto T$ due to $e^{-\theta/\alpha T}$ which tends to unity at high temperatures, which is similar to the earlier finding of Herring [9].

The percentage contribution of three-phonon N and U processes can be analyzed via Figs 3–5. From these Figures, it can be seen that at low temperatures $\tau_{3ph,N}^{-1}$ dominates over $\tau_{3ph,U}^{-1}$ for both transverse and longitudinal phonons. As a result, the three-phonon N-processes play a dominating role in the lattice thermal conductivity. At high temperatures, $\tau_{3ph,U}^{-1}$ dominates over $\tau_{3ph,N}^{-1}$, which shows that the lattice thermal resistivity is mainly due to three-phonon U-processes. These results are similar to those obtained by previous workers [8, 20, 23].

* * *

The author wishes to express his thanks to Dr. W. S. Redda, Dr. R. H. Misho and Dr. K. S. Dubey for their help during the work.

References

1. M. G. Holland, Phys. Rev., *132*, 2461, 1963.
2. C. M. Bhandari and G. S. Verma, Phys. Rev., *140*, A 2101, 1965.
3. R. H. Misho and K. S. Dubey, Indian J. Pure Appl. Phys., *15*, 48, 1977.
4. K. S. Dubey and G. S. Verma, Phys. Rev., *B4*, 4491, 1971.
5. M. C. Al-Edani and K. S. Dubey, Phys. Stat. Sol., (b) *86*, 741, 1978.
6. J. Callaway, Phys. Rev., *113*, 1046, 1959.
7. G. L. Guthrie, Phys. Rev., *152* 801, 1966.
8. K. S. Dubey, J. Thermal Anal., *19*, 1980.
9. C. Herring, Phys. Rev., *95*, 954, 1964.
10. P. C. Sharma, K. S. Dubey and G. S. Verma, Phys. Rev., *B3*, 1985, 1971.
11. K. S. Dubey, Indian J. Pure Appl. Phys., *11*, 265, 1973.
12. K. S. Dubey, Phys. Stat. Sol., *81*, K83, 1977.
13. K. S. Dubey, J. Physique, *37*, 265, 1976.
14. H. B. Casimir, Physica, *5*, 595, 1938.
15. P. G. Klemens, Proc. Roy. Soc. London, *68*, 1113, 1955.
16. I. Pomeranchuk, Phys. Rev., *60*, 82, 1941.
17. I. Pomeranchuk, J. Phys. U.S.S.R., *4*, 259, 1941.
18. M. G. Holland, Phys. Rev., *134*, A471, 1964.
19. Y. P. Joshi and G. S. Verma, Phys. Rev., *B1*, 750, 1970.
20. P. C. Sharma, K. S. Dubey and G. S. Verma, Phys. Rev., *B4*, 1306, 1971.
21. K. S. Dubey and R. H. Misho, J. Therm. Anal., *12*, 223, 1978.
22. K. S. Dubey, Indian J., Pure Appl. Phys., *15*, 455, 1977.
23. A. H. Awad and K. S. Dubey, J. Therm. Anal., *24*, 233, 1982.
24. K. S. Dubey and G. S. Verma, Phys. Rev., *B7*, 2879, 1973.
25. P. G. Klemens, Solid State Physics, ed. by F. Seitz and Turnbull, Academic Press Inc. New York. 7. 1, 1958.
26. P. G. Klemens, Proc. Roy. Soc. London, *A208*, 108, 1951.