Thermal Conductivity and Modification The Formula of The Hole(Electron) – Phonon Scattering: Application to Antimony at Low Temperature

Ahmed. S. Mahdi
(Department of Physics, College of Education, University of Basrah, Iraq)
ISSN 1817 – 2695
((Received 19/1/2010, Accepted 30/6/2010))

Abstract:

Using Callaway's Model, thermal conductivity of antimony in the temperature range between (0.4-2.4)K was calculated. Specialized present study to modification the formula of hole(electron)-phonon scattering relaxation rate by using phonon wave vector which is located in the formula of the hole(electron)-phonon relaxation rate, instead of Debye dispersion relation ($q = \omega / \upsilon$). In addition to scattering the phonons by holes(electrons) ,the boundary scattering, point defects and three-phonon scattering (normal & umklapp) were taken into account to find the total relaxation rate. Good agreement between theory and experiment is obtained in temperature rang (0.4-2.4)K.

Keywords: Thermal Conductivity, Hole(electron)-phonon scattering , Sb

INTRODUCTION:

Thermal conductivity is one of the most fundamental and important properties of material. So, many experimental and theoretical studies on thermal conductivity of solid were worked in recent years[1-4]. In doped semiconductor hole(electron)-phonon relaxation rate plays an important role to decrease the phonon conductivity at low temperature [5-11]. Thermal conductivity depends on the type of doping (p-type or n-type). In p-type semiconductor, hole-phonon scattering relaxation rate plays an important role to find thermal conductivity of semiconductor. The n-type semiconductor of the electron-phonon scattering relaxation rate is ascends for low temperature.

Many studies calculated the thermal conductivity in doped semiconductor, they assumed the phonon wave vector q, as being used among hole(electron)-phonon scattering relaxation rate to be $q = \omega/\upsilon$ (Debye Approximation) and it is correct at the low frequency only [6,10,12-14].

Recently Mahdi[15] studied lattice thermal conductivity in doped semiconductor (p-type InSb ,p-type HgTe and n-type Ge have one charge carriers) by using the equation of the hole(electron)-phonon scattering relation rate modification by using the dispersion relation of diatomic and monatomic lattice instead of Debye approximation ($q = \omega/\upsilon$).

Antimony showed different treatment because it had two types of charge carriers (electron and phonon) in the same time. So, we could take into account the (hole & electron)-phonon relaxation rate together[16]. Consequently the element Sb was analyzed to test the ability of modification the relative of the hole(electron)-phonon scattering relaxation rate having two types of charge carriers in the same time.

Mathematical Description

1-Hole(electron)-phonon scattering

Hole(electron)-phonon scattering in antimony is given by[16]:

$$\tau_{cp}^{-1} = 6\tau_{hp}^{-1} + 3\tau_{ep}^{-1} \qquad (1),$$

Where $\tau_{hp}^{-1}, \tau_{ep}^{-1}$ refer to phonon scattering by hole and electron respectively. There are six hole pockets and three electron pockets in antimony [16],the formula takes the following form:

$$\tau_{h,ep}^{-1}(q) = \frac{m_{h,e}^2 C^2}{2\pi\rho\hbar^3} q \qquad for \quad q \le 2k_F \qquad (2a)$$

$$\tau_{h,ep}^{-1}(q) = 0 \qquad for \quad q > 2k_F \qquad (2b)$$

C is the dilatation deformation potential, $m_{h,e}$ effective hole(electron)-phonon mass, ρ is the mass density , q is the phonon wave vector, and k_F is the radius of the hole Fermi surface.

Phonon conductivity is divided into three ranges of integral[16] :-

(a) $0 < x < \theta_h^*/T$, $\quad \tau^{-1} = \tau'^{-1} + AxT \qquad (3a)$

$$A = \frac{(6m_h^2 + 3m_e^2)C^2}{2\pi\rho\hbar^3 xT} q \qquad (3b)$$

(b) $\theta_h^*/T < x < \theta_e^*/T$, $\tau^{-1} = \tau'^{-1} + A'xT \qquad (4a)$

$$A' = \frac{3m_e^2 C^2}{2\pi\rho\hbar^3 xT} q \qquad (4b)$$

(c) $\theta_e^*/T < x < \theta/T$, $\quad \tau^{-1} = \tau'^{-1} \qquad (5)$, where

τ'^{-1} refer to the scattering of phonon , the parameter $x = \hbar\omega/k_B T$, θ_h^*, θ_e^* effective Debye temperatures of hole and electron respectively.

The first range of integration has accounted for the phonons scattered by holes and electrons. In the second rang the phonons are still scattered by the electron, whereas the third range, accounts for phonons which are scattered by neither of the carriers [16].

2-Other scattering of phonon

Taking the scattering by boundaries τ_B^{-1} ,the charge carriers τ_{cp}^{-1}, point defect τ_{pt}^{-1} and three phonons τ_{3ph}^{-1} where given into account to calculate the total relaxation rate(see table 1) .

Table 1:The formula of the scattering of phonon

Type of scattering	Symbol	Equation	References
Boundary	τ_B^{-1}	υ/L	**[17]**
Point defect	τ_{pt}^{-1}	dx^4T^4	**[18]**
Three phonon scattering	$\tau_{3ph}^{-1} = \tau_N^{-1} + \tau_U^{-1}$	$\tau_N^{-1} = A_n x^2 T^5$ $\tau_U^{-1} = A_u x e^{(\theta/\alpha T)}$	**[19]**

Where υ is the velocity of the sound ,L is the parameter(adj) and α are constant. Characteristic length, d, A_n, A_u adjustable

$$\tau'^{-1} = \tau_B^{-1} + \tau_{ph}^{-1} + \tau_{3ph}^{-1} \qquad (6)$$

3- ***Thermal conductivity***

Thermal conductivity was analyzed by using Callaway's model at low temperature which can be given by[20] .

$$K = \frac{k_B}{2\pi^2 \upsilon}\left(\frac{k_B T}{\hbar}\right)^3 \int_0^{\theta/T} \tau \frac{x^4 e^x}{(e^x - 1)^2} dx \qquad (7)$$

Depending on the assumption (eqs.3, 4 and 5), thermal conductivity can be rewritten in the formula below[16].

$$K = \frac{k_B}{2\pi^2 \upsilon}\left(\frac{k_B T}{\hbar}\right)^3 (I_1 + I_2 + I_3) \qquad (8a)$$

$$I_1 = \int_0^{\theta_h^*/T} (\tau'^{-1} + AxT)^{-1} \frac{x^4 e^x}{(e^x - 1)^2} dx \qquad (8b)$$

$$I_2 = \int_{\theta_h^*/T}^{\theta_e^*/T} (\tau'^{-1} + A'xT)^{-1} \frac{x^4 e^x}{(e^x - 1)^2} dx \qquad (8c)$$

$$I_3 = \int_{\theta_e^*/T}^{\theta/T} \tau' \frac{x^4 e^x}{(e^x - 1)^2} dx \qquad (8d)$$

4- ***Modification of the formula of hole(electron)-phonon scattering relaxation rate***

The dispersion Relation of the monatomic lattice is given by[21]:

$$\omega = \omega_m \sin(qa/2) \qquad (9)$$

We can rewrite(eq.9) the wave number to become:

$$q = \frac{2}{a}\sin^{-1}\left(Tx \Big/ \theta\right), at\ \omega_m = \frac{k_B \theta}{\hbar} \qquad (10)$$

By inserting (eq. 10) into (eqs. 3,4) the expression of the modification proposer takes the formula blow:

(a) $0 < x < \theta_h^*/T$, $\tau^{-1} = \tau'^{-1} + AxT$ (11a)

$$A = \frac{(6m_h^2 + 3m_e^2)C^2}{\pi\rho\hbar^3 xaT}\sin^{-1}(Tx/\theta) \qquad (11b)$$

(b) $\theta_h^*/T < x < \theta_e^*/T$, $\tau^{-1} = \tau'^{-1} + A'xT$ (12a)

$$A' = \frac{3m_e^2 C^2}{\pi\rho\hbar^3 xaT}\sin^{-1}(Tx/\theta) \qquad (12b)$$

Results and Discussion

By using eq.7, thermal conductivity of Sb can be calculated by using the modification proposer (in eqs.11, 12) and eq.5 to find hole(electron)-phonon scattering relaxation rate. The formula of other scattering of phonon in Table 1, and the value of constants in Table 2. The result of the thermal conductivity with temperature can be shown in Fig 1.

Table 2:**Value of constant used to calculate thermal conductivity of Sb in low temperature.**

Constant	Value	Reference
m_e (g)	$0.28\, m_0$	[16]
m_h (g)	$0.14\, m_0$	[16]
$\theta(K)$	210	[16]
$\theta_h^*(K)$	24.4	[16]
$\theta_e^*(K)$	30.8	[16]
α	1.8	adj
$C(e.V)$	0.32	adj
A_N	1.0×10^{-11}	adj
d	3.07	adj
$\tau_N^{-1}(s^{-1})$	3.5×10^{-7}	adj
A_u	2.7×10^{6}	adj
$\upsilon(cm.\sec^{-1})$	2.2×10^{5}	adj
$a(A^o)$	4.49	[22]
$\rho(gm.cm^{-3})$	6.69	[22]

Solid line in Fig 1 represents the theoretical curve and the experimental results has been got from three references[16,23,24] in compile to have temperature ranged from 0.4K - 4.2K.

From Fig.1 (the dash line), it can be seen that the hole(electron)-phonon scattering relaxation rate plays an important role to calculate thermal conductivity (Specialize above 1K), because the boundary scattering relaxation rate controlled to other scattering in the temperature (below 1K).

Fig.2 shows the importance of modification of the formula of hole(electron)-phonon scattering relaxation rate in different values of thermal conductivity after and before the modification, by using parameter in the present paper and compute it (see Table 2).

Deferent percentage was found between thermal conductivity after and before modification to show the importance of the modification on total thermal conductivity by using the formula below, to put the result in Table 3.

$$\%K = \frac{K' - K''}{K''} \times 100\% \qquad (13)$$

Where K', K'' represent the thermal conductivity after and before modification respectively.

Table 3: Deferent percentage between thermal conductivity vs. temperature after and before modification.

T(K)	%K
0.4	17.78
0.6	25.00
0.8	31.22
1.0	43.09
1.2	45.51
1.4	48.38
1.6	53.57
1.8	58.00
2.0	62.24
2.2	66.53
2.4	70.52

The results of Table 3 show the importance of modification as it arrived the top percentage value 70.52% (at T=2.4K) because of the dominate hole(electron)-phonon scattering relaxation rate on other scattering. So the modification causes high effect on the thermal conductivity. If temperature range begins to drip, falling percentage value to 17.78% (for T=0.4K) can be seen because of the increasing the effect of the boundary scattering .

In the present study abatement contribution of point defect scattering and three phonon scattering to the total relaxation rate can be noticed in the two range(first and second relaxation rate) because of the low temperature range(see Fig. 3). In the third range, hole(electron) -phonon relaxation rate(eq.5) disappeared and begin point defect scattering to dominate in high frequency(see fig. 4).

The value of $\alpha, C, \tau_B^{-1}, d, A_N, A_u, \upsilon$ (in table 2) it consider the adjustable parameter (adj) to get the fitting between the experimental and theoretical results.

Conclusion

Based on theoretical result of the thermal conductivity, the hole(electron)-phonon scattering can be noticed to play an important role to calculate total thermal conductivity in Sb (Specialize above 1K). So it is necessary to take this scattering into account to find thermal conductivity.

Differences between theoretical curve after and before modification the formula of the hole(electron)-phonon scattering relaxation rate were found it is necessary to take into account to find thermal conductivity more delicate.

The ability to change the relation of the monatomic lattice ($q = \frac{2}{a}\sin^{-1}(Tx/\theta)$) instead Debye approximation ($q = \omega/\upsilon$) correctly in low frequency was noticed in samples having two charge carriers (electron and phonon) in the same time ,after applying it successfully to samples having one charge carriers only[15].

It can be seen from a results a good fitting between experimental and theoretical thermal conductivity resulted in the low temperature range.

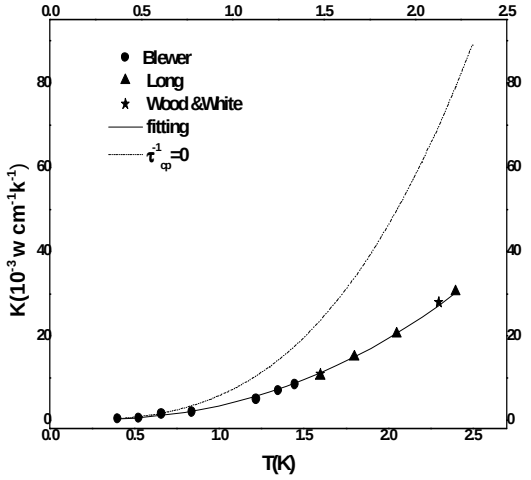

Fig 1: Thermal Conductivity vs. Temperature from 0.4-4.2 K

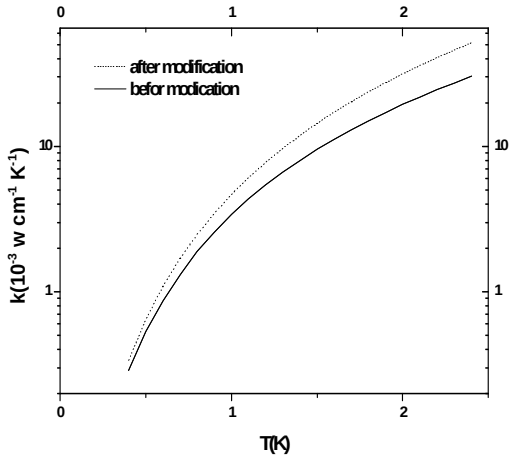

Fig 2:The different thermal conductivity after and before rearrangement of the formula of hole(electron)-phonon scattering relaxation rate.

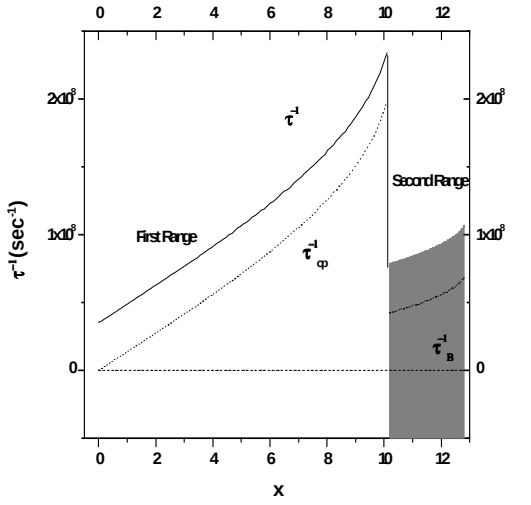

Fig 3: relaxation rate vs. parameter x (at T=2.4K) in first and second range

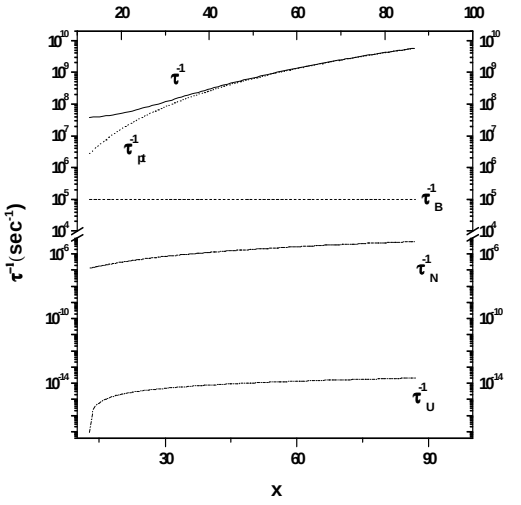

Fig 4: relaxation rate vs. parameter x (at T=2.4K) third range

References

1. R. Lal et al. **Physica C** 469,106(2009).
2. Xue-Qian Fang, **Applied Thermal Engineering** 29,925(2009).
3. M. Chandrasekar et al, **Experimental Thermal and Fluid science** 34, 210 (2010).
4. D. Pinisetty and R. V. Devireddy ,**Acta Materialia** 58, 570(2010).
5. C. R. Whitett and D. A. Nelson**, Phys. Rev**. B5, 8(1972).
6. K. Suzuki and N. Mikoshiba, **Phys. Rev.** 3, 2550(1971).
7. B. L. Bird and N. Pearlman**, Phys. Rev. B**4, 4406(1971).
8. M. Singh, **Phys. Rev. B**18, 2950(1978).
9. M. Singh, **Phys. Rev**. 23, 2983(1981).
10. A. H. Awad, **J. of Thermal Analysis and Calorimetry** Vol. 63, 597(2001).
11. A. H. Awad, **Pure Sciences**,Vol 27, 99 (2000).
12. J. M. Ziman, **Philos. mag**. 1,192(1956);2, 292 (1957).
13. V. V. Kosarev, P. V. Tamarin and S. S. Shalyt, **Phys. Stat. Sol**, (b)44,525(1971).
14. C. R. Crosby and C. G. Grenier, **Phys. Rev. B** 4, 1258 (1971).
15. A. S. Mahdi, M. Sc. Thesis, Basrah University, Basra (Iraq) 2007.
16. R. S. Blewer, N. H. Zebouni and C. G. Grenier, **Phys. Rev.** 174,700(1968).
17. H. B. Casimir ,Physica, 5, 595 (1938).
18. P. G. Klemens, **Solid State Physics** 7, edited by F. Seitz and D. Turnbull, Academic Press, New York, 1 (1958).
19. C. Herring, **Phys. Rev**. 95, 954(1954).
20. J. Callaway, **Phys. Rev**.113,1046 (1959).
21. C. Kittel. *Introduction to Solid State Physics*, 2^{nd} Edition, John Wiley and Sons, Inc.New York(1976).
22. M. Wakaki ,K. Kudo and T. Shibuya *Physical Properties and Data of Optical Materials*(2007).
23. J. R. Long, C. G. Grenier, and J. M. Reynolds, **Phys. Rev. 140,A187** (1965) .
24. G. K. White and S. B. Woods, **Phil. Mag**. 3, 342(1958).

الخلاصة:-

باستخدام نموذج كالوي تم حساب التوصيل الحراري للانتيمون في مدى حراري يتراوح بين 0.4 الى 2.4 درجة مطلقة . خصصت الدراسة لتعديل العلاقات الخاصة بالمعدل الزمني للاسترخاء للتشتت الفونوني بالفجوات او الالكترونات باستخدام علاقة المتجه الموجي للفونون الموجودة ضمن علاقة التشتت الفونوني بالفجوات او الالكترونات بدلاً من علاقة التفريق لديباي($q = \omega / \upsilon$) .تـم الاخـذ بالاعتبار التشتت الفونوني بحدود البلورة وبالعيوب البلورية وبالفونونات الثلاثية (الاعتيادية والاومكلابية) لحساب المعدل الكلي لـزمن الاسترخاء. تم الحصول على تطابق جيد بين القيم العملية والنظرية للتوصيل الحراري.