Lattice Thermal Conductivity of Solid Neon

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ABSTRACT

The lattice thermal conductivity of solid neon has been calculated over the temperatures range (0.5-10 K), at molar volume (13.4 cm^3/mole) by using Awad model. Taking into account five types of scattering mechanisms boundary, dislocation, point defects, isotopes and three phonon scattering. Good agreement with the experimental data achieved by using adjustable parameters, maximum conductivity value reached to (307 mW/cm.K) at (3.1 K).

Keywords: Thermal conductivity, Solid neon, Law temperature.

INTRODUCTION

Rare-gas crystals are probably the simplest dielectric solids which can study the phonon heat transport and the role of boundary, dislocations, point defects, the three phonon and other scattering mechanisms, in order to compare the theoretical analysis with the experimental results $[1-3]$.

Solid neon is one of the simplest crystals with regard to crystal structure, lattice dynamics, and other physical properties, and because of several interesting properties, was, and still is, subjected to intense study of many authors$[4-8]$.

Kimber and Rogers [9] studied the thermal transport properties of solid mixtures for the neon isotopes ^{20}Ne and ^{22}Ne. The results have been interpreted numerically by using the Callaway formulation[10] to establish the relaxation rates of the phonon scattering. They were found the phonon scattering by isotopic impurity atoms (40%) stronger than the predicted on the basis of the mass difference alone.

Clemans [11] studied the thermal conductivity of solid neon sample, measured through the temperature range (0.5-10 K). An isotopically purified ^{20}Ne sample, and a ^{20}Ne sample with 0.15-at. % ^{4}He, as well as a sample with the natural isotopic mixture, were studied. Callaway relaxation rate theory[10] was used to make a good agreement with experimental data[9].

Awad[12] progressed mathematical model exceeding all the approximations used by Callaway[10] or any earlier authors, by using dispersion relation of monatomic and diatomic lattices, he has taken accounts both of dispersion relation for sound phonons and non equilibrium distribution function consequent at interaction with the nearest and all atoms. He got more accurate formulas in order to calculate the lattice thermal conductivity. He applied these formulas in successfully on Germanium Ge and Gallium Arsenide GaAs in the temperatures range (2-300 K).

Because of the theoretical studies dearth on this sample, which has been considered one

of the impediment essential, in order to compare with, so the purpose of the present work is to calculate the lattice thermal conductivity of isotopic purified solid neon ^{20}Ne theoretically at the temperature range (0.5-10 K) by using Awad model [12] to get best fitting with the experimental data[11].

Mathematical description

The measurement results were analyzed by using the method of Awad[12], who worked in his investigation to discuss all the approximations used by earlier authors[10, 13 − 18], and treatment it mathematical at calculating the lattice thermal conductivity of solids, where he obtained formulas of the lattice thermal conductivity and correction term for the following states as:

I. Dispersion relation

Awad[12] ignored Debye approximation of dispersion relation ($q = \omega/v$), which is used by Callaway method[10], and he used in his model the dispersion relation of monatomic lattice in one dimension as[19] :

$$\omega = \omega_m \sin\left(\frac{\bar{q}a}{2}\right)$$

So, he was getting to the following formula for the lattice thermal conductivity and correction term as:

$$k = k_1 + \Delta k$$

$$k_1 = c\theta I_1$$

$$I_1 = \int_0^{\theta/T} \tau_C \frac{x^2 e^x}{(e^x-1)^2} \sqrt{1-(Tx/\theta)^2}\left(\sin^{-1}(Tx/\theta)\right)^2 dx$$

Where, θ is Debye temperature, and k_1 represents the conductivity if the normal processes scattering are small, while

$$\Delta k = c\theta I_2 I_4 / I_3$$

is included when normal processes are significant.

$$I_2 = \int_0^{\theta/T} \frac{\tau_C}{\tau_N} \frac{xe^x}{(e^x-1)^2}\left(\sin^{-1}(Tx/\theta)\right)^3 dx$$

$$I_3 = \int_0^{\theta/T} \frac{1}{\tau_N}\left(1-\frac{\tau_C}{\tau_N}\right) \frac{e^x}{(e^x-1)^2} \sqrt{1-(Tx/\theta)^2}\left(\sin^{-1}(Tx/\theta)\right)^4 dx$$

$$I_4 = \int_0^{\theta/T} \frac{\tau_C}{\tau_N} \frac{xe^x}{(e^x-1)^2}(1-(Tx/\theta)^2)\left(\sin^{-1}(Tx/\theta)\right)^3 dx$$

$c = \left(\frac{k_B^3 T}{3\pi^2 a\hbar^2}\right)$, $x = \frac{\hbar\omega}{k_B T}$, $\theta = 75.1$ K, $\alpha = 2.3$ [11], $a = 4.46\ A^o$ [19].

τ_C : The combined relaxation time, given by:

$$\tau_C^{-1} = \tau_B^{-1} + \tau_{pt}^{-1} + \tau_D^{-1} + \tau_{3ph}^{-1} + \tau_I^{-1}$$

$$= \frac{v}{l} + A\omega^4 + B_D\omega T + \left(B_N + B_U e^{-\theta/\alpha T}\right)\omega^2 T^3 + B_I \omega^4 T^4$$

Where, $\tau_B^{-1}, \tau_{pt}^{-1}, \tau_d^{-1}, \tau_{3ph}^{-1}\ and\ \tau_I^{-1}$ are relaxation time for the boundary, point defect, dislocation, three phonon and isotope scattering, respectively.

ω : The phonon frequency.

II. Non-equilibrium distribution function

To correct the lattice thermal conductivity equation, Awad used non

equilibrium distribution function by treating the deflecting magnitude of equilibrium distribution function $N^O(t)$ [20] as:

$$N(t) = N^O(t) - \int_{-\infty}^{t} d\acute{t}\, e^{\frac{\acute{t}-t}{\tau}} \frac{d}{d\acute{t}} N^O(\acute{t})$$

Where,

$N(t)$: Non equilibrium distribution function in time period t.

$N^O(t)$: Equilibrium distribution function in time period t.

$N^O(\acute{t})$: Equilibrium distribution function in time period $\acute{t}$.

t : Time period after scattering process.

$\acute{t}$: Time period before scattering process.

So, the lattice thermal conductivity and correction term has been written as [12] :

$$k = c_o \frac{\theta}{C_v}\left[I_5 + \frac{I_2 I_6}{I_3}\right]$$

Where, the first term represents the thermal conductivity, while the second term represents the correction term.

$$I_5 = \int_0^{\theta/T} \tau_C \frac{x^3 e^x}{(e^x-1)^2} \sqrt{1-(Tx/\theta)^2}\left(sin^{-1}(Tx/\theta)\right)^2 dx$$

$$I_6 = \int_0^{\theta/T} \frac{\tau_C}{\tau_N} \frac{x^2 e^x}{(e^x-1)^2} (1-(Tx/\theta)^2)\left(sin^{-1}(Tx/\theta)\right)^3 dx$$

$$C_v = \frac{4V_O k_B T}{\pi^2 a^3 \theta} \int_0^{\theta/T} \frac{x^2 e^x}{(e^x-1)^2} \frac{\left(sin^{-1}(Tx/\theta)\right)^2}{\sqrt{1-(Tx/\theta)^2}} dx$$

$$c_o = \left(\frac{k_B^4 T}{3\pi^2 a \hbar^2}\right) .$$

RESULTS AND DISCUSSION

The lattice thermal conductivity of solid neon calculated for both states of dispersion relation and non equilibrium distribution function by using the adjustable parameters of the phonon scattering appearing in tables (I,II), the results represented in figures (1,5). Best fitting can be noticed of these results with experimental data[11], especially at the maximum conductivity curve. But some abnormalities can be found of these theoretical calculations about the experimental data for this sample at relatively high temperature through the range (5-7 K), which can be treated by using the two mode conducting theory. In the same figures (1,5), the results of the earlier authors Kimber and Rogers[9] were also included.

The point defect phonon scattering included and should be considered carefully, for the significance important at solidified the sample, the previous study did not take that account[11], and that significance can be seen in figures (2,6), The phonon scattering processes of the point defects, boundary and dislocation show the domination at low temperatures, but the isotopic and three phonon scattering of two kinds (normal and umklapp processes) dominate at high temperatures.

In figures (3,7), the normal processes of three phonon scattering were dominant at temperature less than (4 K), but at high temperatures the umklapp processes were dominant, this is an agreement with the results of authors $[21-23]$.

At constant temperature (T= 3.1 K) and within low frequencies range, the figures (4,8) appearing dominance for the boundary and dislocation phonon scattering over another kinds of scatters, on the other hand the isotopic and point defects scattering dominion at high frequencies, this is an agreement with the results of the authors $[12,24-26]$.

CONCLUSIONS

The lattice thermal conductivity of solid neon has been measured over the temperature range (0.5-10 K). Awad method has been applied to analyze the obtained data. The point defect phonon scattering has been included, and it is important at temperatures below (4 K).

The calculated values of the lattice thermal conductivity through the temperatures range (5-7 K) higher than the experimental one, especially in dispersion relation state, but these abnormalities contracted in non equilibrium distribution function state.

The boundary and isotopic phonon scattering play important roles in the lower and higher frequencies consecutively.

Table I: The adjustable parameters values calculated and used for theoretical curves.

τ_B^{-1}	1.05×10^{3}	s^{-1}
A	1.0×10^{-46}	s^{3}
B_D	3.5×10^{-10}	deg^{-3}
B_N	0.1×10^{-23}	deg^{-3}
B_{II}	0.36×10^{-20}	deg^{-3}
B_I	0.6×10^{-47}	deg^{-3}

Table II: The adjustable parameters values calculated and used for theoretical curves.

τ_B^{-1}	1.5×10^{3}	s^{-1}
A	0.1×10^{-46}	s^{3}
B_D	5.5×10^{-10}	deg^{-3}
B_N	0.1×10^{-24}	deg^{-3}
B_U	0.9×10^{-21}	deg^{-3}
B_I	0.25×10^{-46}	deg^{-3}

The figures (1-4) for dispersion relation state.

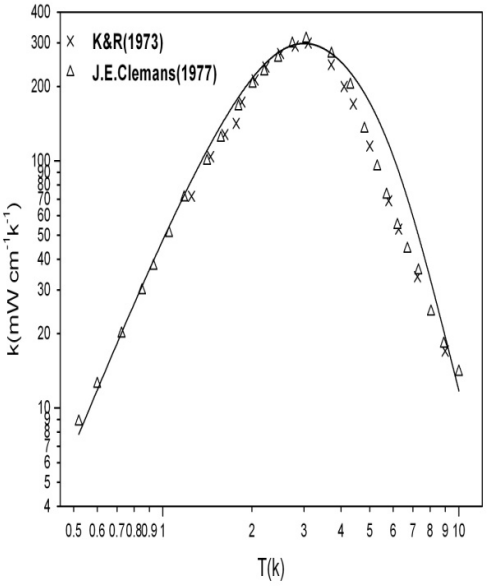

Fig.1: Conductivity curves of solid neon. Solid line is the present work.

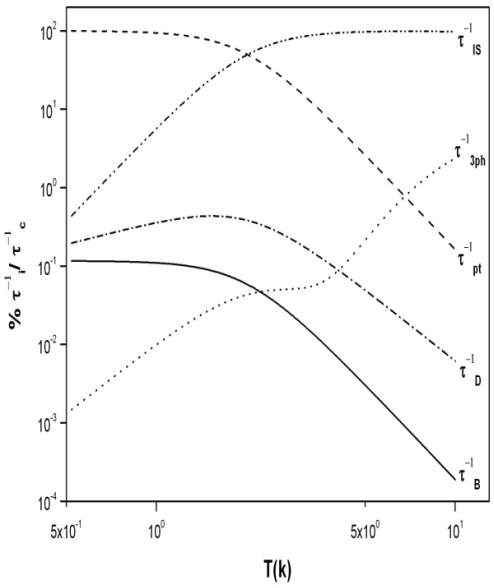

Fig.2: The percentage contribution of relaxation rates scattering used towards the combined relaxation rate.

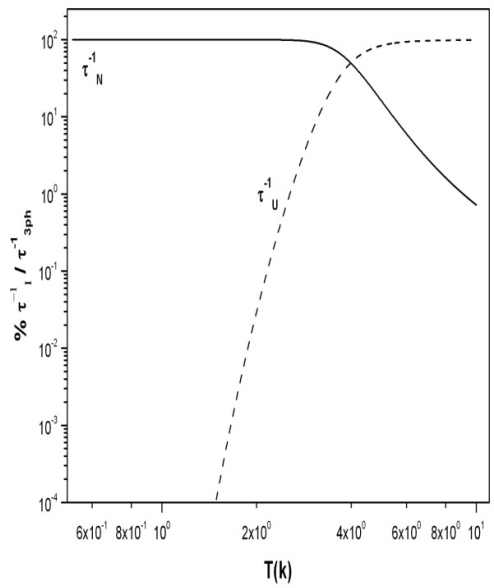

Fig.3: The percentage contribution for the relaxation rate of normal and umklapp processes towards the relaxation rate of three phonon scattering.

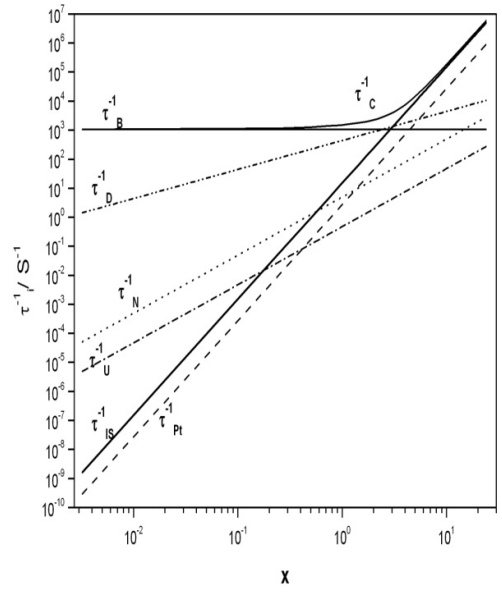

Fig.4: Relaxation rates of the deferent phonon scattering as a function to the factor x at constant temperature.

The figures (5-8) for non equilibrium distribution function state.

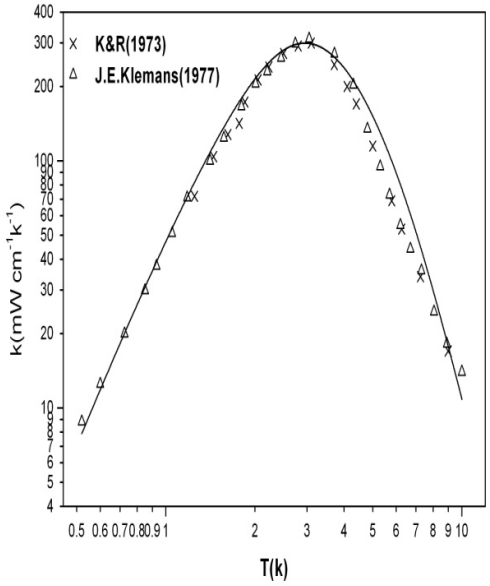

Fig.5: Conductivity curves of solid neon. Solid line is the present work.

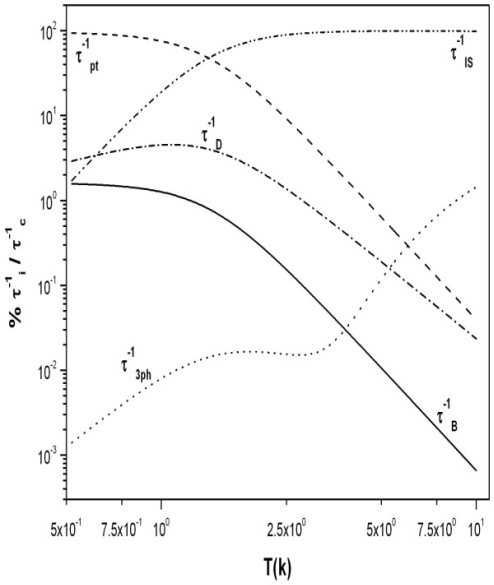

Fig.6: The percentage contribution of relaxation rates scattering used towards the combined relaxation rate.

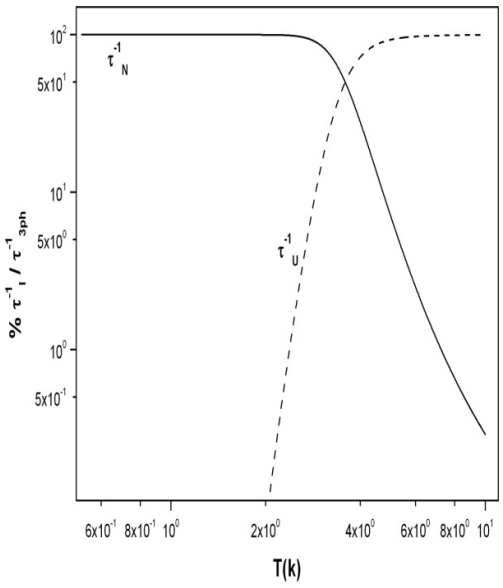

Fig.7: The percentage contribution for the relaxation rate of normal and umklapp processes towards the relaxation rate of three phonon scattering.

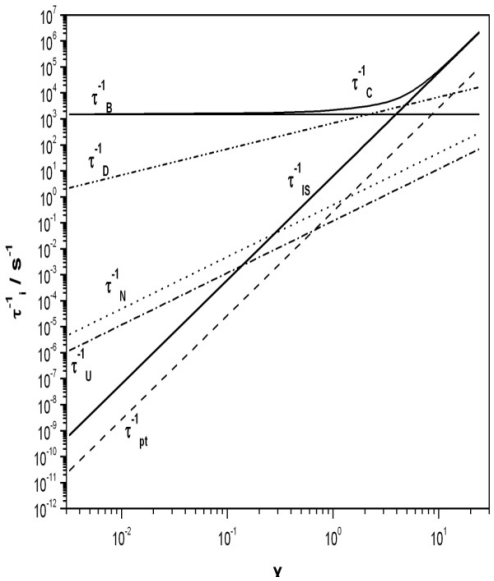

Fig.8: Relaxation rates of the deferent phonon scattering as a function to the factor x at constant temperature.

REFERENCES

[1] V. A. Kostantinov, V. G. Manzhely, M. A. Strzhemechnyi, and S. A.

Smirnov, **Sov. Low Temp. Phys.** 14,48 (1988).

[2] D. N. Batchelder, **in Rare Gas Solids,** edited by M. L. Klein and J.

A. Vanables (Academic, London, Vol. 2.(1977).

[3] G. K. White and Woods, **Philos. Mag.** 3,785 (1958).

[4] C. L. Julian, **Phys. Rev.** 137, 128 (1965).

[5] D. B. Benin, **Phys. Rev. Lett.** 20, 1352 (1968).

[6] B. J. Bennett, **Solid State Commun.** 8, 65 (1970).

[7] H. T. Weston and W. B. Daniels, **Phys. Rev. B**29, 2709 (1984).

[8] C. Cazorla[1,2] and J. Boront[3], **Phys. Rev. B**77, 024310 (2008).

[9] R. M. Kimber and S. J. Rogers, **J. Phys. C**6, 2279 (1973).

[10] J. Callaway, **Phys. Rev.** 113, 1046 (1959).

[11] J. E. Clemans, **Phys. Rev. B**15, 1072 (1977).

[12] A. H. Awad, **Ph. D. Thesis,** Basrah University, Basrah (Iraq)

(2003).

[13] M. G. Holland, **Phys. Rev.** 132, 2461 (1963).

[14] Y. P. Joshi and G. S. Verma, **Phys. Rev. B**1, 750 (1970).

[15] P. C. Sharma, K. S. Dubey and G. S. Verma, **Phys. Rev. B**3, 1985

(1971).

[16] A. H. Awad, **Acta Physica Hungarica** 72,115 (1992).

[17] M. D. Tiwari and B. K. Agrawal, **Phys. Rev. B**4, 3527 (1971).

[18] K. S. Dubey, **Phys. Stat. Solidi** (b) 63, k35 (1974).

[19] C. Kittel, **Introduction to Solid State Physics,** 6th ed. John Wiley

and Sons, Inc, New York (1986).

[20] N. W. Ashcroft and N. D Mermin, **Solid State Physics,** Saunders

College, 248 (1975).

[21] A. H. Awad, **Acta Physica Hungarica** 63, 331 (1988).

[22] A. H. Awad, **J. of Thermal Analysis** 39, 559 (1993).

[23] A. H. Awad and Q. H. A. Hussain, **Engineering and Technology**

13, 7 (1994).

[24] A. J. Mohammed, **M. Sc. Thesis,** Basrah University, Basrah (Iraq)

(2007).

[25] A. S. Mehdi, **M. Sc. Thesis,** Basrah University, Basrah (Iraq)

(2007).

[26] D. B. Habesh, **M. Sc. Thesis,** Basrah University, Basrah (Iraq)

(2008).

ملخص

تم حساب التوصيل الحراري الشبيكي للنيون الصلب في مدى درجات الحرارة (0.5–10) درجة مطلقة، وذلك باستخدام نموذج عواد. وقد أخذت بنظر الاعتبار خمسة أنواع من تشتتات الفونونات عن حدود البلورة والخلع البلوري والعيوب النقطية والنظائر والتشتتات الفونونية الثلاثية. وقد تبين إن هناك تطابقاً جيداً بين القيم التجريبية والقيم المحسوبة، كما إن أعلى قيمة للتوصيل الحراري تصل إلى (307 ملي واط / سم . درجة مطلقة) عند درجة الحرارة (3.1) درجة مطلقة.