MODEL OF PHONON CONDUCTIVITY FOR MAGNESIUM STANNIDE

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ABSTRACT

Due to its peculiar properties, the non metallic solids have been important elements in the semiconductor device industry. Particularly, the estimation of phonon conductivity of such solids becomes important for their applications. Magnesium Stannide (Mg_2Sn) is one of the such elements in the present study to analyses the phonon conductivity. In the presence of the interaction term which dominants near the low temperature and the exponential temperature dependence which dominants significantly at the higher temperature. In the estimation of the phonon conductivity, the inter-dependence of the relaxation rates, due to isotopic impurities ($\tau^{-1}_D \sim A\omega^4$) and anharmonic interactions ($\tau^{-1}_A = B\omega^2T^3$) has been considered in the form of a cross term (I^{AD}). The present study investigates the role of the cross term (in explaining the low temperature lattice thermal conductivity, of solids, doped with isotopic impurities) and the exponential temperature dependence of the parameter (due to its significant role at high temperature) have been analyzed using the model on the computer. A good agreement has been achieved with experimental data nearly up to 70K which validates the model computed on computer.

Keywords: Computer Applications, Model, Magnesium Stannide, Phonon Conductivity

I. INTRODUCTION

The non metallic solids have been important elements in the semiconductor device industry. Particularly, the estimation of phonon conductivity of such solids becomes important for their applications. Magnesium Stannide (Mg_2Sn) is one of the such elements which has been analyzed in the present study by measuring is conductivity. Doped with isotopic impurities, the estimation of phonon conductivity of non metallic solids has been an important application area in the semiconductor device industry. Because of their wide applications, measuring of thermal conductivity of these solids has been a great interest among the researchers[1-4]. The present work analyses the thermal conductivity of intrinsic semiconductor, of which the transport behavior is similar to the insulator with heat conduction due to lattice waves i.e. phonons. The present study does not consider the electronic contribution in the thermal conductivity measurement. The model given by Callaway[5] has been used to by above mentioned researchers particularly for the low temperature range. In the measurement of phonon conductivity, they have directly assumed that the relaxation rates due to isotopic impurities ($r^{-1}_D \sim A\omega^4$) and anharmonic ($r^{-1}_A = B\omega^2T^3$) are independent of each other, which are then added in accordance with

Mathiessen's rule and that there is no interference or cross term of defect with anharmonic parameters, appearing in the total phonon relaxation time. in estimating the thermal conductivity of doped crystals, this cross term (r^{AD}) cannot be ignored in the exact calculations, particularly near the low temperature maximum , where the conventional domination of r^{-1}_{D} ends and that of r^{-1}_{A} starts. The present paper investigates the role of this cross term, in explaining the low temperature lattice thermal conductivity, of solids, doped with isotopic impurities. In addition, exponential temperature dependence of the parameter B_2 as discussed below has also been taken into account due to its significant role at high temperature as proposed by Gairola[6]. For conduction calculations, computer aided simulation approach has already been in use e.g. Osetsky[7] has applied simulation to study the high temperature phase stability in iron, a good conductor. The proposed model is also simulated with modified steps by Bhatt and Gairola[2] in the preliminary work on semiconductors taking account the basic method mentioned by Gordon [8] and Avil[9]. The following sections discuss the phonon conductivity model, results, analysis and lastly the conclusion.

II. PHONON CONDUCTIVITY MODEL

In analyzing the phonon conductivity of Mg_2Sn, as measured earlier by Martin and Danielson[10] up to 50^0K, the present estimation is done in the temperature range 4 – 82^0K, using the simulation approach, as described by Bhatt and Gairola[9] to achieve consistency with the experimental results. It has been a usual practice, to generally neglect the exponential temperature dependence of the parameter B_2, representing Umklapp phonon-scattering and both B_1 (normal phonon scattering parameter) and B_2 are lumped into single parameter B, assumed to be independent of T, as considered earlier by Bhatt and Gairola[11] for the analysis of Ge. This is because, at low temperature B_2 does not change significantly with T but at higher temperature it changes considerably. Therefore, B_2 is taken to depend upon T, exponentially, as has also been considered by Martin and Danielson[10], in analyzing conductivity of Mg2Sn. Their theoretically analyzed curve, however, shows poor agreement above 50^0K. In the present study, the effect of the change in B1 has also been analyzed. In the following sub-sections, modeling and simulation has been discussed.

2.1. Modeling

As the present analysis is rigorous and involves less approximation in comparison to other models, therefore, simulation techniques has been applied on the mathematical model as proposed by Gairola[12] which a modified version of Callaway's model[5] and being iteratively computed. The following equation shows the mathematical/computational model taken for the simulation process :

$$\tau^{-1} = v/FL + A\omega^4 + [B_1+B_2 \exp.(-\Theta/aT)]\ \omega^2 T^3 + D\ \omega^3 T \qquad \ldots(1)$$

This mathematical model as shown by the Eq.-1 above, has been computed for the estimation of phonon conductivity of Mg_2Sn in the temperature range 4 – 90 K considering the previous approach [9]. In this Computation, out of several responses, only relevant response has been considered which shows similar experimental values.

2.2. Simulation

There are five stages[9] which are selectively mapped-out for computer-based simulation process viz. entities/attributes & activities; system image & routine; simulation procedure; report generation & storing; and interaction interface. In the last phase, the flow of simulation process is being interacted by assigning new values of parameters/attributes in the model so as to find the experimental results[14]. So in achieving such useful simulated responses, arithmetic and logical conditions have been applied and manipulated to decide to accepted or neglected the simulated responses. These responses have been discussed in the following section.

III. RESULT

On the basis of above defined methodology, the model is being simulated and suitable responses have been gathered as shown in the Table-1 and Table-2. Nine parameters have been assigned the values as shown in the Table-1.

Table-1: Parameters

Parameters	Values
v	359 cm/sec
L	.11
F	.54
α	2.5
Θ_D	154
A	6.3×10^{-44} sec^3
B_1	7.7×10^{-23} sec K^{-3}
B_1	4.7×10^{-23} sec K^{-3}
D	2.75×10^{-33} sec^3 K^{-1}

Using these values of nine parameters, phonon conductivity has been measured at 14 different stages of the temperature in the range of 4 – 90^0K. Following Table-2 shows the corresponding to the results for the conductivity for each stage of the temperature taken.

Table-2: Phonon Conductivity

Temperature (Kelvin)	4	6	8	10	14
Conductivity ($Wcm^{-1}K^{-1}$) x 10^7	0.9672	2.374	3.878	5.125	6.296
Temperature (Kelvin)	20	26	30	36	40
Conductivity ($Wcm^{-1}K^{-1}$)	5.322	3.592	2.710	1.818	1.425

x 10^7					
Temperature (Kelvin)	50	60	70	82	90
Conductivity ($Wcm^{-1}K^{-1}$) x 10^7	0.837	0.539	0.372	0.255	0.2050

The results of the Table-2 have been graphically represented in the Fig.-1; where experimental points have been marked as circles and the present study with the solid line. In the present investigation, the role of the cross term (in explaining the low temperature lattice thermal conductivity, of solids, doped with isotopic impurities) and the exponential temperature dependence of the parameter B_2 (due to its significant role at high temperature) have been analyzed.

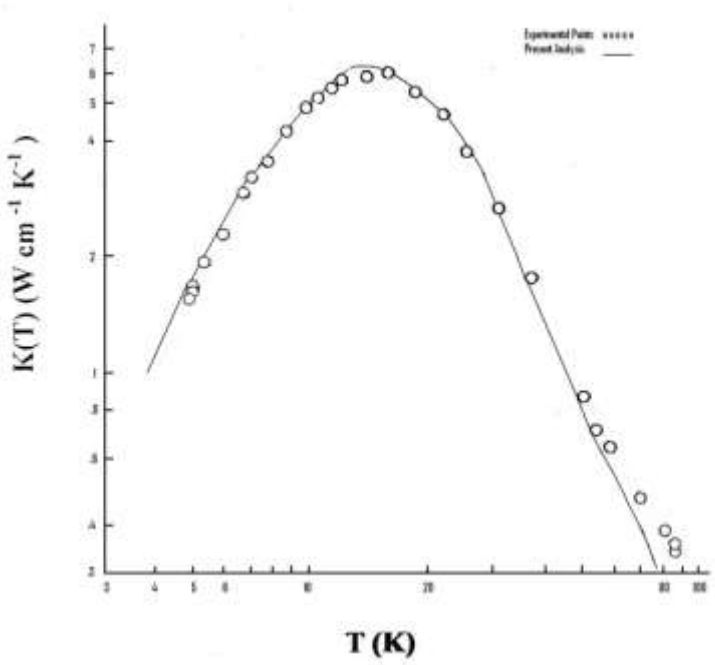

Fig.-1: Phonon Conductivity Of Mg_2Sn

It is evident from the Fig.-1, that a good agreement has been achieved with experimental data up to 60^oK. This validates the role of these terms in the proposed model. Further, the simulation process also optimizes the approach of the conductivity estimation. Further, it has also been observed from the previous work[16] that by decreasing the B1 parameter from 7.7 to 7.0 in the present case, at lower and higher temperature ranges that up to 20K and above 30K onwards no any much deviation in the conductivity values have been noticed but a significant variations have been observed in the mid temperature range i.e. from 20 to 30K.

V. CONCLUSION

The present study concludes that the existence of the interaction term dominants near the low temperature and the exponential temperature dependence which dominants significantly at the higher temperature; which is

apparently depicts from the result and the figure. On comparing these results, significant observations are being notices near the mid range of temperature.

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