Theoretical Calculations of the Temperature and Impurity Dependence of the Lattice Thermal Conductivity for the $ZnSnAs_2$ Semiconductor Compound

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Abstract

The Callaway models are used to calculate lattice thermal conductivity for $ZnSnAs_2$ Semiconductor in the temperature range (2—300) K. The dependence of lattice thermal conductivity on temperature and impurity concentration as well as the strength of scattering are discussed, The maximum thermal conductivity for elven samples investigated are appears at the temperature 21K. is 3.54 W/cm.K,This reduces to 0.093 W/cm.K for impurity concentrations from $0.21x10^{20}$ cm^{-3} to $3x10^{21}$ cm^{-3}. The scattering strength is also investigated and found to be equal to -0.7203.

Keywords:- $ZnSnAs_2$ Semiconductor, Lattice Thermal Conductivity, Carrier Concentration relaxation time.

Introduction

$ZnSnAs_2$ is the ternary semiconducting compound which belongs to the group II-IV-V_2 is analogises to the binary III-V compound semiconductors [1]. Differential thermal analysis and the X-ray diffraction showed that this compound transforms from chalcopyrite to disordered zink blende structure at 650 C^o where its melting point is 775C^o [2]. Its optical energy gap has been reported to be equal to 0.6 eV [2], and also its variation with temperature has been investigated [3]. Its Debye temperature and the volume expansion coefficient have been found as 268 K.and 6.9 x 10^{-6} K^{-1}respectively [4,5] The thermal and electrical properties have been investigated experimentally in some detail [2,6].

This work represents the effect of the temperature as well as impurity concentration on the lattice thermal conductivity for eleven samples of the ternary $ZnSnAs_2$ semiconductor compound.

Theoretical aspects

The lattice thermal conductivity for the ternary $ZnSnAs_2$ semiconductor compound can be calculated by the approximation solution to the Boltzmann transport equation

in the relaxation time approximation. According to the models developed by Callaway [7] which is refined by Holland [8], the value of the lattice "phonon" thermal conductivity is determined by the integral over the phonon spectrum as:

$$K_l = \frac{1}{3}\int_0^{\omega_d} S(\omega)\tau_c(\omega)v_g^2 d\omega \quad \ldots\ldots(1)$$

Where $S(\omega)d\omega$ is the specific heat per unit volume due to lattice modes of frequency $\omega, d\omega$ and $\tau_c(\omega)$ is their effective "combined" relaxation time , ω_d is the Debye frequency and v_g is the average phonon group velocity which is given by[9].

$$v_g^{-1} = \frac{1}{3}\left(\frac{1}{v_l} + \frac{2}{v_t}\right) \quad \ldots\ldots(2)$$

hence v_l and v_t are the longitudinal .and transverse velocities respectively and they are a function of phonon frequency [10]. When the dominant process is the resistive process which do not conserve crystal momentum. Then K_{ph} can be calculated through the Callaway expression [7,10-15]:

$$K_l = \frac{k_B}{4\pi^2 v_g}\left(\frac{k_B}{\hbar}\right)^3 T^3 \int_0^{\frac{\theta_D}{T}} \frac{\tau_c x^4 e^x}{(e^x-1)^2} dx \quad ..(3)$$

where K_B is the Boltzmann constant , $\hbar$ is the Plank's constant, θ_d is the Debye temperature ,$x = \frac{\hbar\omega}{k_B T}$ and τ_c is the combined relaxation time, and which can be given by :

$$\tau_c^{-1} = \sum_i \tau_i^{-1} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (4)$$

hence τ_i ,s are the relaxation times for the individual processes, According to the Mathiessens rule. the process can be limited to only three major contributions in the temperature region (2-300) K as:

$$\tau_c^{-1} = \tau_b^{-1} + \tau_u^{-1} + \tau_i^{-1} \quad \ldots\ldots(5)$$

where τ_b, τ_u and τ_i are the relaxation times due to the boundary , Umklapp and mass difference or isotopes scattering respectively. However the latter is due to the presence of atoms having a mass different from the average atomic mass forming the compound, and from the isotopes of a particular element in the compound or may be due to the existence of impurity atoms.

The boundary scattering is treated by using the Casimir limit assumption [16], in the form of relaxation time as:

$$\tau_b^{-1} = \frac{v_g}{FL} \quad \ldots\ldots\ldots\ldots\ldots\ldots(6)$$

where F has the value of unity [17], L is the characteristic length for the bulk sample which can be calculated by Casimir formula[18],and its value found to be equal to 0.41915 cm, The group velocity v_g can be calculated from the equation[19]:

$$v_g = \frac{k_B\theta_D}{\hbar}\left(\frac{V}{6\pi^2}\right)^{\frac{1}{3}} \ldots\ldots\ldots\ldots (7)$$

Where V is the average atomic volume which is equal to 2.505 x 10^{-23} cm^{-3} for $ZnSnAs_2$,and with the value of θ_D as 268 K[4].then v_g will get the value of 2.634 x 10^5 cm/sec.

The inverse relaxation time due to Umklapp process has been proposed by Slack and Galginaitis [20] as:

$$\tau_c^{-1} = B_2\ \omega^2 T e^{-\frac{\theta_D}{\alpha T}} \ldots\ldots\ldots\ldots\ldots(8)$$

where $B_2 = \frac{\hbar\gamma^2}{Mv_g^2\theta_D^2}$ and its value is equal to 3.44 x 10^{-18} sec.K^{-1}, where γ and M are the Gruneisen constant having values of 2.9[17] and 83.522 a.m.u. respectively. The parameter α which is depends on the dispersion and the elastic anisotropy of the lattice wave, is also related to the phonon energy spectrum as well as the structure of the brillouin zone for phonons [17]. For a simple Debye model it is assumed to have the value of 2 [21].

For Rayleigh- type scattering of phonons by point defects "isotope", The expression for the relaxation time will be[22]:

$$\tau_i^{-1} = A\omega^4 \quad \text{.....(9)}$$

where parameter A is the isotope strength which is the sum of at least two terms of A_{iso} and A_{imp} , A_{iso} is due to the scattering of phonons by isotopes, that is from departure from the perfect periodicity in the lattice. The compound $ZnSnAs_2$ is contains sixteen isotopes five for Zn, ten for Sn and one for As. A_{iso} can be calculated through the equation[22]:

$$A_{iso} = \frac{V}{4\pi^2 v_g^3}\left[\sum_i f_i\left(1-\frac{M_i}{M}\right)\right] \text{.....(10)}$$

$$\Gamma = \sum_i f_i\left(1-\frac{M_i}{M}\right)^2$$

when f_i is the relative abundance of the i^{th} isotope and M is the average mass of the species , then Γ found to have the value of 6.518 x 10^{-45} which gives the value for A_{iso} to be 7.1 x 10^{-45} sec^3 , The difference in the stiffness constant between the impurity-host atoms, as well as the difference in the atomic volumes for impurities, are also be included in the phonon scattering rate expression[13],Then the expression which for scattering due to these point defects "A_{imp}" is given by the relation [17]:

$$A_{imp} \frac{3V^3 N_{imp}}{\pi v_g^3} \quad \text{.....(11)}$$

where N_{imp} is the sum of the concentrations of imperfection, such as vacancies, interstitial cation and anion antisite disorders and other foreign atoms. By assuming N_{imp} to be equal to the carrier "hole" concentration for these samples, the value of $A=A_{iso}+A_{imp}$ can be calculated as shown in the table below:

Sample no.	N_{imp} x$10^{20}$$cm^{-3}$	Ax$10^{-42}$$sec^3$
K1	0.21	0.6957
K2	0.85	2.794
K3	1.4	4.598
K4	3.0	9.845
K5	4.4	14.43
K6	5.7	18.7
K7	6.4	21
K8	8.1	26.57
K9	8.9	29.19
K10	20	65.59
K11	33	108.2

Result and Discussion

Results for the lattice thermal conductivity as a function of temperature for eleven samples of $ZnSnAs_2$ having different carrier concentration are plotted in fig (1).

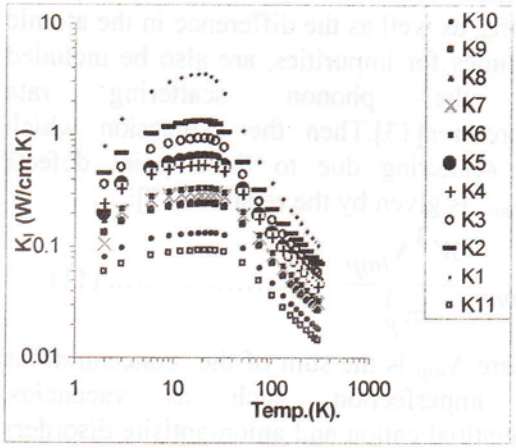

Fig.(1) Variation of the thermal conductivity with temperature for eleven samples of $ZnSnAs_2$ with different impurity concentration using equ.(3).

The maximum lattice thermal conductivity [23] for semiconductor generally located at the place between the Umklapp and boundary scattering region which is occur at T=21K for this compound, However the appearance of K_{max} perhaps is one of the most striking predictions of quantum theory of solids [24],it is also very sensitive to the effect of impurities, carrier concentration and imperfections .These are creates extra scatters for the phonons which is consequently gives rise to extra thermal resistance[25,26] .At such a temperature and to a large extent the high–frequency phonon are not excited . It is reasonable to use the factor τ_i^{-1} in the form $\tau_i^{-1} = A\omega^4$ this is particularly valid for the low frequency phonons [27], The height of the peak which is governed by isotope scattering [24] is affected by the impurity concentrations according to the relation $K_{\max} \approx N_{imp}^{-\chi}$ [27],where χ is the scattering strength. The impurities in the ranges of ($0.21x10^{21}$ cm^{-3} - $33x10^{21}$ cm^{-3}). for $ZnSnAs_2$ gives K_{max} to changes according to $K_{max} \approx N_{imp}^{-0.7203}$ which is illustrated in fig (2).

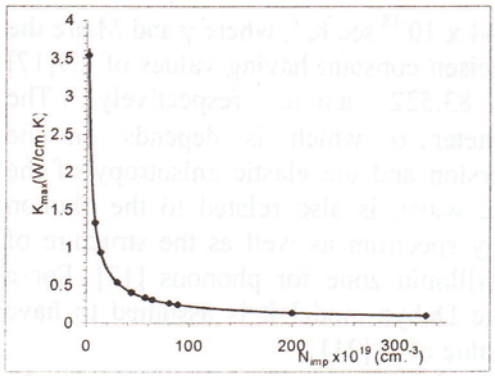

Fig.(2) The maximum lattice thermal conductivity for $ZnSnAs_2$ as a function of impurity concentration at 21K.

Figure (3) shows the temperature dependence of χ which is changes according to the relation $\chi = 1.7405\ T^{-0.2913}$ for the temperature up to 140K and as $\chi = -3x10^{-4}$ T+0.4852 for temperature above that.

However the latter is explained the convergence of the thermal conductivity curves to be due to impurity concentration compared to that of the K_{max} location.

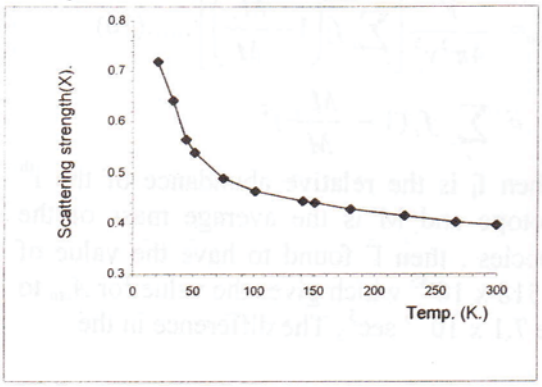

Fig.(3) Temperature dependence of the scattering.

Conclusion

1. The Callaway model, which is suitable for calculating lattice thermal conductivity for most crystalline solids, is given suitable results for the ternary semiconducting compound $ZnSnAs_2$ ternary.

2. The maximum lattice thermal conductivity is affected strongly by impurity and decreases with it according to the equation $K_{max} \approx N_{imp}^{-0.7203}$.

3. The impurity scattering strength decreases with increasing temperature and it effect appears strongly at temperature 100 K.

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پێوانەی تیۆری تۆرە گەیاندنی گەرمی لە پێکهاتەی نیمچە گەیەنەری $ZnSnAs_2$ لەنێوان پلەی گەرمی (٢-٣٠٠) کلڤندا

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پوختە

مۆدێلی کالاوای بەکارهات بۆ پێوانەکردنی تۆرەگەیاندنی گەرمی لەنیمچەگەیەنەری $ZnSnAs_2$ لەنێوان (٢-٣٠٠) کلڤندا , وە گۆڕانی تۆرە گەیاندنی گەرمی لەگەڵ پلەی گەرمیو چڕی خڵتەدا هەروەها توندی لادان باس کران وە بەرستری گەیاندنی گەرمی دەکاتە ٣,٥٤٣ وات /سم.کلڤن لەپلەی ٢١ کلڤندا وە دە گۆڕێت بۆ ٠,٠٩٣ وات /سم.کلڤن بۆ چڕی (٠,٢١ X 10^{20} تا ٣,٢ X 10^{21}) سم $^{-3}$ وەبڕی توندی لادان یەکسانە بە (٠,٧٢٠٣-) ە.

دراسة نظرية للتوصيلية الحرارية الشبيكة للمركب شبه الموصل $ZnSnAs_2$ لمدى الحرارى (٢٠٠-٣٠٠) كلفن

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الخلاصة

استخدمت نموذج كالاواى لحساب التوصيلية الحرارية الشبكية للمركب شبه الموصل $ZnSnAs_2$ لمدى الحرارى (٢-٣٠٠) كلفن .وتم مناقشة اعتماد التوصيلية الحرارية مع درجة الحرارة وتركيز الشوائب اضافة على شدة الأستطارة ، وتبينت ان اعلى توصيلية الحرارية حوالي (٣,٥٤٣ واط /سم.كلفن) عند درجة ٢١ كلفن ويتغير الى ٠,٠٩٣ واط /سم.كلفن للتركيز من (٠,٢١ X 10^{20} الى ٣,٢ X 10^{21}) سم $^{-3}$ وقيمة شدة الاستطارة تساوى (٠,٧٢٠٣-).

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