



THERMAL CONDUCTIVITY OF Cr –DOPED GaAs AT LOW TEMPERATURE

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ABSTRACT

The thermal behavior of solids changes drastically due to presence of stacking fault dislocations present in the crystals. These faults offer considerable thermal resistance at low temperature and in addition to the thermal boundary resistance, the significant contribution to the thermal transport of solids cannot be ignored. The inverse relaxation time of phonons scattered from stacking faults vary as the square of phonon frequencies and linearly with the dislocation density. The study of lattice thermal conductivity of GaAs containing the Chromium dislocations has been made at low temperatures. After inclusion of internal boundary scattering of phonons it gives good agreements with the experimental values. A modified form of Callaway model has been used in calculating the thermal conductivity.

Keywords: *Boundary Scattering, Dislocations, Internal-External Boundary, Microboundary, Relaxation Time, Stacking Faults*

I. INTRODUCTION

Study of specific type of defects in GaAs has been made in a number of papers [1-4]. Chromium doped GaAs is semi insulating solid and is a very good electric and optoelectric device. Chromium doping is a convenient and very reliable method for producing semi-insulating Gallium Arsenide Crystals [5]. Vuillermoz et.al [6] obtained several Cr:GaAs samples. Structural disorder or some defect can also exist during the crystal growth. Usually, the existing dislocations in a face centered cubic crystal may split into two types of partial dislocations: A plane separating two halves of the crystal which has been displaced by sliding, so that there is a thin but highly sheared region between the two half planes. This type of thin sheet of dislocation is known as stacking fault. These stacking faults in [111] orientation has been observed by experimentalists and have been discussed in their experimental details [6, 7]. They have tried to justify the experimental data for the lattice thermal conductivity theoretically but could not succeed.

In the present paper the experimental details of Vuillermoz show that the stacking faults show the resistivity greater than 10^7 ohm cm in [111] orientations. This suggests that the stacking faults present in the specimen heavily affect the thermal transport at low temperatures. Also, development of these dislocations increases the possibility of misfits and micro scale fluctuations in crystal micro boundaries. The relaxation time is a significant part of the Callaway theory of thermal conductivity [8]. The scattering of phonons from stacking faults, external and internal (micro) boundaries [10, 11] of the crystals and from point imperfections (defects) then may contribute a lot towards thermal transport at low temperatures in the present case.



II. THEORY

The stacking fault interactions are associated with the relaxation time

$$\tau^{-1}_s = 0.7(d\gamma\omega)^2 N/v \tag{1}$$

Where N is the number of stacking faults per cm, γ is the Gruneisen constant (=2), v is phonon velocity and d is the lattice parameter.

Casimir [11] in his original paper developed the theory of boundary scattering relaxation rate assuming perfect roughness of the crystals ignoring all other phonon process. This theory has been modified [9,10,12] by considering partially reflecting , partially absorbing and partially rough surfaces which would make changes in the crystal micro boundaries and develops the strains inside the crystals to grow internal boundaries. The internal boundaries appear due to the large microscale fluctuations in the crystal composition. Due to the creation of microboundaries the phonon mean free paths will certainly be shortened and the boundary scattering relaxation time, here in after called the internal-external boundary (IEB) relaxation time τ_{IEB}^{-1} can be given by [9]

$$\tau^{-1}_{IEB} = \frac{v}{L(B)} \tag{2}$$

With $L(B) = 1.12 l B(I)$, here $l = (l_1 l_2)^{1/2}$ with l_1, l_2 as cross sectional areas of the specimen and

$$B(I) = 1.7858 t^{-1}(t_1^{-1} + t_2^{-1})^{-1} \tag{3}$$

l is known as internal boundary parameter (micro boundary parameter) t_1 and t_2 are small timing taken by phonons to traverse a length l forward and backward, respectively in the presence of other scattering so that t_1 may be or may not be equal to t_2 . T is the time taken by phonons to traverse the length l in absence of internal boundaries and other phonon processes. Evidently t is always less than t^1 and t^2 , here $B(I)$ is used as a parameter.

The point defect scattering can be defined by the relaxation rate

$$\tau^{-1}_{pr} = A\omega^4 \tag{4}$$

Where

$$A = \frac{V_o}{4\pi v^3} \sum f_i \left(1 - \frac{M_i}{M}\right)^2 \tag{5}$$

Here V_o is the atomic volume, f_i the fraction of atoms of mass M_i and M is the average atomic mass. The lattice thermal conductivity can be given by expression [8]

$$K = \frac{K_B^4 T^3}{2\pi^2 v \hbar^3} \int_0^{x_D} \tau_c x^4 e^x (e^x - 1)^{-2} dx \tag{6}$$

Where $x_D = \theta/T$, $x = \frac{\hbar\omega}{K_B T}$ and the combined relaxation time

$$\tau_c^{-1} = \tau_{IEB}^{-1} + \tau_s^{-1} + \tau_{pr}^{-1} + \tau_{3ph}^{-1} \tag{7}$$

$\tau_{3ph}^{-1} = B\omega^2 T^3$ is the phonon-phonon relaxation time. At low temperatures the boundary scattering relaxation time is highly dominating term and the other terms contribute much less. Following this argument the equation (6) can be written as



$$K = \eta \int_0^{x_D} \tau_c x^4 e^x (e^x - 1)^{-2} [1 + \beta x^2 + \alpha x^4]^{-1} dx \quad [8]$$

Where,

$$\eta = \frac{K_B^4 T^3}{2\pi^2 v h^3} \quad [9a]$$

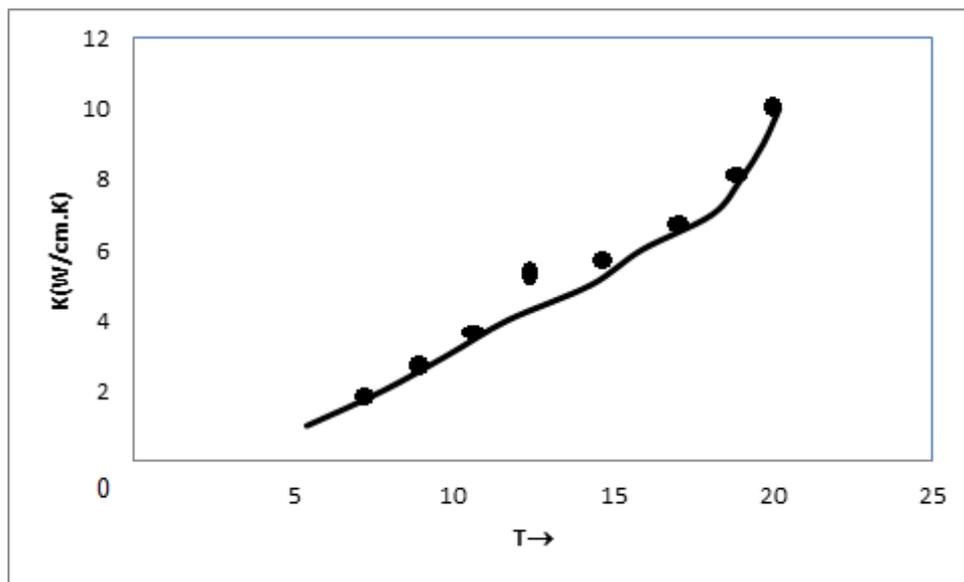
$$\alpha = \frac{AL(B)K_B^4 T^4}{v h^4} \quad [9b]$$

$$\beta = \frac{L(B)K_B^2 T^2}{v h^2} \left[BT^3 + \frac{.7(d\gamma)^2 N}{v} \right] \quad [9c]$$

At very low temperatures, due to high value of Debye temperature θ the upper limit $x_D \rightarrow \infty$ and the conductivity expression takes the form-

$$K = \eta [\xi(4) - \beta \xi(6) - (\alpha - \beta) \xi(8)] \quad [10]$$

Where $\xi(n)$ are the Reimann Zeta functions.



GRAPH: Lattice Thermal Conductivity of Cr doped GaAs at low temperatures

- Experimental values
- Full curve Theoretical fit

III. DISCUSSIONS

The lattice thermal conductivity of Cr doped GaAs has been analysed with the help of expression given in equation (10). The number of dislocation has been taken 185 cm^{-1} . The parameter casimir length $L = .25$, $v = 3.3 \times 10^5 \text{ cm} \cdot \text{sec}^{-1}$, $\gamma = 2.0$, $d = 5.65 \text{ \AA}$, $B(I) = 7.6 \times 10^{-3}$, $A = .51 \times 10^{-44} \text{ sec}^{-3}$ have been taken for analysis. The theoretical analysis presented here on the basis of above expressions give appreciable agreement with experiments in the temperature region under consideration. In the analysis it has been observed that the IEB was dominant during the low temperature region.

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