

STUDY OF EFFECTIVE DEBYE TEMPERATURE FOR PURE AND DOPED *n*-TYPE GALLIUM ANTIMONIDE

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ABSTRACT

The effect of *n* doping on Debye temperature θ and maximum frequency ν_m of a compound (III and V group) semiconductor named 'gallium antimonide' has been studied at temperatures below 300° K from two different theoretical approaches which make a good use of the second order elastic moduli. The results obtained from both the methods are in good agreement with each other.

INTRODUCTION

THE single parameter theory of specific heat given by Debye¹ explains the observations remarkably well. It's one parameter Debye temperature θ can now be evaluated by using SOEM data in the place of heat capacity measurements. In the previous paper we have dealt with the determination of θ for NaCl using the two different theoretical approaches namely de Launay² and Betts *et al.*³ methods at different temperatures and pressures. Here, to know the effect of doping on Debye temperature θ , we have studied a pure and doped semiconductor gallium antimonide (GaSb) at different temperatures. The purpose of the present paper is three fold: first to evaluate the Debye temperature at various temperatures, second to know the doping effect on it and third to compare the relative merits and demerits of both the methods used.

THEORY

Considering the solid to be an elastic continuum the Debye temperature θ for solids has been defined as⁴

$$\begin{aligned} \theta &= \frac{h}{k} \nu_m = \left(\frac{9N}{4\pi V} \right)^{1/3} \\ &\times \frac{h}{k} \cdot \left[\int \left(\frac{1}{C_1^3} + \frac{1}{C_2^3} + \frac{1}{C_3^3} \right) \frac{d\Omega}{4\pi} \right]^{-1/3} \end{aligned} \quad (1)$$

where ν_m is the maximum Debye frequency possible in a system, $d\Omega$ is the element of solid angle, C is the velocity, N is the Avogadro's number and V is the volume. Calculation of θ from the above equation is not easy since it involves solving a cubic equation and then finding the average value of a function of these roots.

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de Launey, later on, considered a cubic lattice of Born Von Karman⁵ type with central forces connecting the nearest and next nearest atoms and simplified above expression in terms of density and second order elastic constants and added the contribution due to the compressibility of the electron gas. The simplified expression thus obtained for Debye θ in terms of second order elastic constant is,

$$\theta = \frac{h}{k} \left(\frac{9N}{4\pi V} \right)^{1/3} \left(\frac{C_{44}}{\rho} \right)^{1/2} \left(\frac{9}{18 + \sqrt{3} f} \right)^{1/3} \quad (2)$$

where $f_{(s, \nu)}$ ⁶ is a function of the elastic anisotropy of the crystal and other terms have their usual meanings.

Vonderlage and Bethe⁷ replaced the integral in eq. (1) in terms of the cubic harmonics $K_m(\theta, \phi)$ of order m as

$$I(\theta, \phi) = \sum_m a_m K_m(\theta, \phi) \quad (3)$$

where θ and ϕ specify a particular direction in the lattice and the suffix m represents the number of crystallographic directions chosen. This model was proposed by Houston⁸ for the directions $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$ and was used by Bhatia and Tauber⁹ in the calculation of θ . Betts *et al.* later on extended this upto six terms by adding the direction $\langle 210 \rangle$, $\langle 211 \rangle$ and $\langle 221 \rangle$ and obtained an expression of θ in terms of second order elastic constants as,

$$\theta = \frac{h}{k} \left(\frac{9N}{4\pi M} \right)^{1/3} \rho^{-1/2} J(4)^{-1/3} \quad (4)$$

where $J(4)$ is the linear combination of I_1, I_2, I_3, I_4, I_5 and I_6 which are recognised as the $\rho^{-3/2}$ times the integrand in the Debye expression evaluated in the above six directions.

RESULTS AND DISCUSSION

Wong and Lin¹⁰ measured the temperature dependence of second order elastic constants of pure

TABLE I

Temperature dependence of effective Debye temperature and maximum Debye frequency of GaSb

Temp. °K	θ^* °K	θ^{**} K	ν_m^*	ν_m^{**}	$\eta = \frac{2C_{44}}{C_{11} - C_{12}}$
Pure GaSb					
4.2	268.81	269.86	560.06	562.25	1.7961
100	268.38	269.51	559.16	561.52	1.7941
140	267.95	268.70	558.27	559.82	1.7956
180	267.28	268.00	556.87	558.37	1.7970
220	266.55	267.30	555.35	556.92	1.7966
260	265.94	266.72	554.08	555.71	1.7960
300	265.39	266.14	552.94	554.50	1.7948
Doped GaSb					
4.2	268.81	269.63	560.06	561.77	1.7953
100	268.38	269.16	559.16	560.79	1.7939
140	267.83	268.35	558.02	559.10	1.7938
180	266.92	267.30	556.12	556.91	1.7948
220	266.34	267.22	554.91	556.75	1.7946
260	265.94	266.44	554.08	555.16	1.7940
300	265.21	265.79	552.56	553.77	1.7922

* By de Launey's method.

** By method of Betts *et al.*

(*p*-type) and doped (*n*-type) gallium antimonide. Both samples have carrier concentrations of the order of 10^{17} cm^{-3} . Using de Launay and Betts *et al.*, methods we have evaluated the values of effective Debye temperature, θ , and maximum Debye frequency, ν_m , of both the samples at different temperatures and the results obtained are reported in Table I. Table I, also reports the values of elastic anisotropy η at different temperatures. By comparing the results of these samples, we can see how much effect doping has on θ , ν_m and η .

It is clear from the Table that the values of parameters θ , ν_m and η show a general decrease with doping which is very small. The values of θ and ν_m of pure and doped GaSb obtained from both the methods decrease with temperature. It is interesting to note that the values of ν_m obtained from both the methods are in excellent agreement with each other, the difference being not more than 0.37% throughout the range of temperature investigated.

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