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Preasure Variation of Debye Temperature and Gruneisen Constant.

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Abstract: *Debye theory of specific heat. has the dimensions of temperature and is defined by* $\theta = h\nu/k$, *where h is the Planck constant, ν is the maximum frequency for the lattice vibrations of the solid, and k is the Boltzmann constant. The Debye temperature is characteristic of the particular material;.*
A new empirical expression is developed to calculate the Debye characteristic temperature of cubic crystals. The calculated Debye temperatures for cubic crystals are shown to be in excellent agreement with other existing computations as well as with the experimental values.

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I. Introduction

Debye temperature is the phenomena which sums of the entire lattice. Also it is known as cahrecteristic temperature of the material. It characterizes numerous properties of solids, such as specific heat, elastic conductivity, thermal conductivity, broadening of x – ray spectral lines and elastic properties. It was introduced by Peter Debye to estimate the contribution of phonon to the specific heat of a solid.

Debye is defined as $\theta_D = \frac{h\nu}{K}$, h is the planck's constant, ν is the frequency and k is the Boltzman constant.

At low temperature mode of vibration of atoms is very small and wavelength can easily predict the low temperature dependence of heat capacity , which is proportional to T^3 law and $T << T_D$

T high temperature vibration of atoms are very large therefore frequency of vibration is too high it obeys Dulong Pettit law. It accounts for anharmonic vibrarion of solids.

When $T >> T_D$ $\frac{Cv}{NK} = 3$

Debye theory is unable to explIN Heat capacity of Liquids because liquids sustin only longitudinal phonons. Neutron scattering experiments insist for the some vibrational existanct of Phonons..

II. Method

The definition of Gruneisen constant is

$$\Upsilon = \frac{d\log\ \nu}{d\log\ \nu} \qquad (1)$$

Assuming with Gruneisen that volume
e variation is same for all frequencies, so we can write that

$$\Upsilon = \frac{d\log\ \nu_D}{d\log\ \nu} \qquad (2)$$

Where ν_D now is the Debye Frequency. We can work in terms of Debye temperature ($\theta_D = \frac{h\nu_D}{K}$) and pressure variation instead of volume variation. Equation (2) may be written as

$$\Upsilon = \frac{B}{\theta_D}\frac{d\theta_D}{dP} \qquad (3)$$

Where B is the bulk modulus. Equation (3) affords a method of evaluation of Υ from pressure variation of Debye temperature. There is hardly any information on the pressure variation of Debye temperature. Kumari and Das (1984) have theoretically considered the pressure variation of Debye temperature. They have obtained the following equation for Debye temperature in terms of Pressure.

Temperature at $\frac{\theta_P}{\theta_D} = (1+\frac{\Upsilon P}{B})$ (4)

It can be easily seen that this equation is the integral form of equation .(3). Kumara and Das (1984) calculated the Debye temperature of Na Cl different pressure using the above equation, but commented that experimental data on pressure variation of Debye temperature is not available to verify their equation.

Recently Sirdeshmukh and Subhadra (1988) have studied the pressure variation of Debye temperature of crystals with Na Cl structure. They calculated the Debye temperatures from the data on elastic constant at high pressure. Such calculations have not been done for crystals with CaF_2 structure. Since, data on the pressure variation of elastic constants are available for several crystals with CaF_2 structures . we have undertaken the calculation of Debye temperature as a function of Pressure. From these results Gruneisen constant has been estimated using equation (3).

For these calculations of Debye temperature and from elastic constant, the method of Betts et al (1956), with eight term approximation has been utilized. The relevant formulas used for this purpose are mentioned below.

$$\Theta = \left(\frac{h}{k}\right)\left(\frac{9s}{A}\right)^{1/3} \rho^{-1}/_2 \; J^{-1}/_3$$

$$J = \frac{4\Pi}{1081080}\left[117603 I_A + 76544 + 17496\, I_C + 381250\, I_D + 311040\, I_E + 177147\, I_F\right]$$

$$I_A = \frac{3}{2}\, 2\langle C_{44}\rangle^{\frac{-3}{2}} + [C_{44} + \propto]^{\frac{-3}{2}}$$

$$I_B = \frac{3}{2}\,\langle C_{44}\rangle^{\frac{-3}{2}} + \left[C_{44} + \frac{1}{2}\,(\alpha - \beta)\right]^{\frac{-3}{2}} + \left[C_{44} + \frac{1}{2}\,(\alpha + \beta)\right]^{\frac{-3}{2}}$$

$$I_C = \frac{3}{2} + 2\left[C_{44} + \frac{1}{3}\,(\alpha - \beta)\right]^{\frac{-3}{2}} + \left[C_{44} + \frac{1}{3}\,(\alpha + 2\beta)\right]^{\frac{-3}{2}}$$

$$I_D = \frac{3}{2}\,[C_{44}]^{\frac{-3}{2}} + \left[C_{44} + \frac{1}{2\propto} + \frac{1}{10}(9 \propto^2 + 16\beta^2)^{\frac{1}{2}}\right]^{\frac{-3}{2}} + \left[C_{44} + \frac{1}{2\propto} - \frac{1}{10}(9 \propto^2 + 16\beta^2)^{\frac{1}{2}}\right]^{\frac{-3}{2}}$$

$$I_E = \frac{3}{2}\left[C_{44} + \frac{1}{6}\,(\propto -\beta\right]^{\frac{-3}{2}} + \left[C_{44} + \frac{1}{12}(5 \propto +\beta) + \frac{1}{12}\,(9 \propto^2 + 3\beta^2 - 6 \propto \beta)^{\frac{1}{2}}\right]^{\frac{-3}{2}}$$

$$I_F = \frac{3}{2}\left[C_{44} + \frac{4}{9}(\propto -\beta)\right]^{\frac{-3}{2}} + \left[C_{44} + \frac{1}{18}\,(5 \propto +9\beta) + \frac{1}{18}\,(9 \propto^2 48\beta^2 + 24 \propto \beta)^{\frac{1}{2}}\right]^{\frac{-3}{2}} + \left[C_{44} + \frac{1}{18}(5 \propto +4\beta - 118(9\propto 2 + 48\beta 2 + 24\propto\beta)12 - 32\right.$$

Where A is cell volume
S is number of atoms /unit cell
$\propto$ is $(C_{11} - C_{44})$
β is $(C_{12} + C_{44})$
P is density
h and k have the usual significance.

Table ---- (1)
Pressure variation of Debye Temperature

S.No	P.(Kbar)	CaF_2	SrF_2	BaF_2	CdF_2	PbF_2
1	0	504.74	374.11	20.83	313.71	218.23
2	1	505.44	374.51	281.01	317.41	218.54
3	2	506.13	374.91	281.18	315.10	218.85
4	3	506.84	375.31	281.35	315.79	219.16
5	4	507.54	375.72	281.53	316.47	219.46
6	5	508.22	376.11	281.70	317.16	- - -
7	6	508.91	375.51	281.88	317.84	- - -

Table ----- (2)
γ from pressure variation of θ

S.No	Crystal	CaF_2	SrF_2	BaF_2	CdF_2	PbF_2
1	Θ_0	504.7	374.1	280.8	313.7	218.2
2	$Kx10^2$(KB)	8.40	7.13	5.84	10.54	6.03
3	$d\theta/_{dp}\,(K\ bar)$	0.695	0.40	1.175.	0.688	0.307
4	γ from equation (3)	1.16	0.76	0.36	2.32	0.84
5	$\gamma_{thermal}$	1.74	1.63	1.66	2.30	2.08

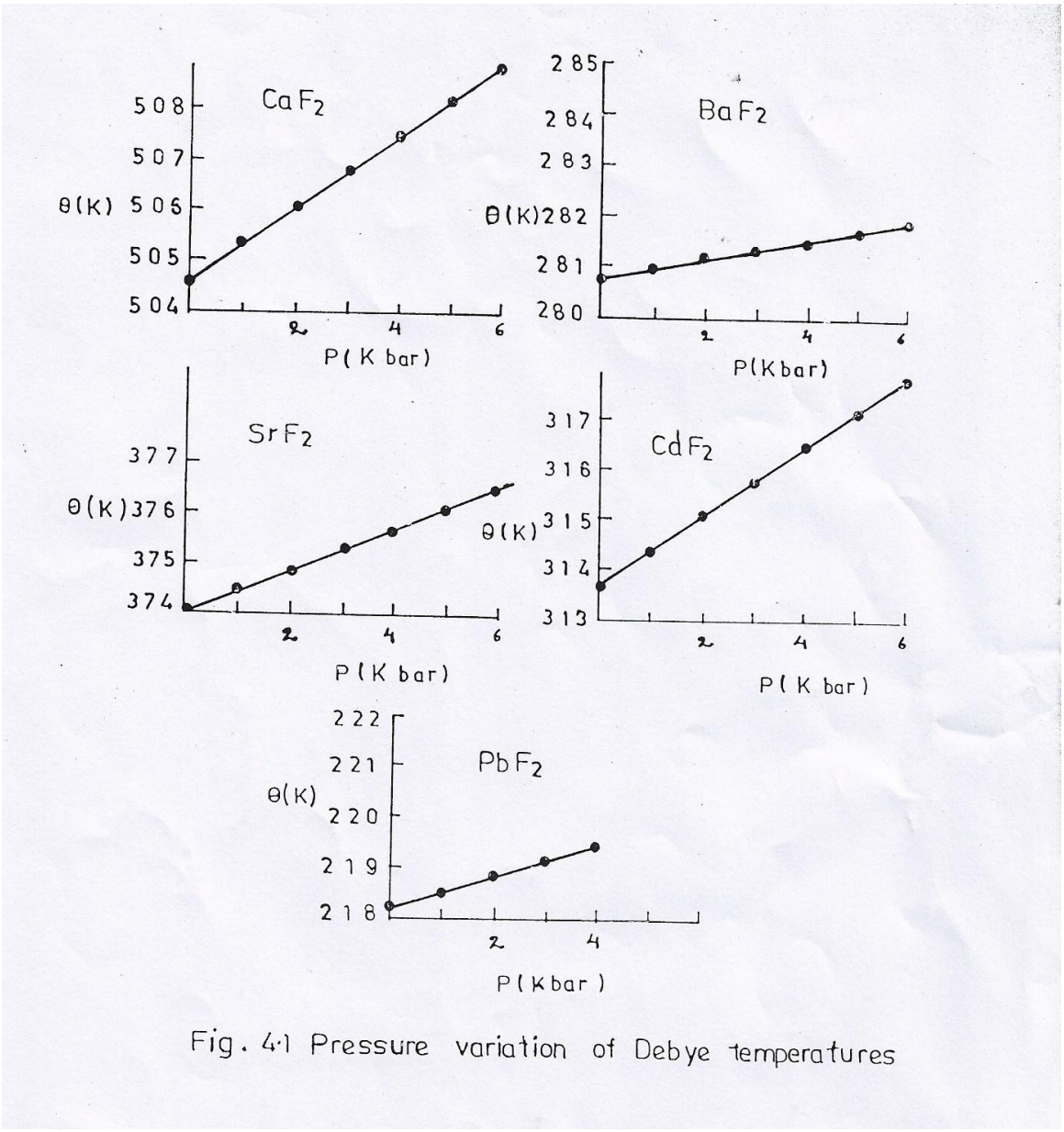

Fig. 4.1 Pressure variation of Debye temperatures

III. Result And Discussion

The values of Debye temperature at various pressures for five crystals are given in table (1). As observed by Sirdeshmukh and Subhadra (1988), the pressure variation of Debye temperature is a small effect. In figure (1), the Debye temperature is shown as function of pressure. It may be seen that for all the five crystals the pressure variation is linear. The values of the Gruneisen constant calculated from the pressure variation of Debye temperature are given in table (2) along with the thermal values. It may be seen that

i) There is an order- of- magnitude between the two sets of values.
ii) These values are systematically lower than theoretical values and
iii) The agreement is very good in in CdF_2, moderate in CaF_2 and poor in BaF_2.

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