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Temperature Variation of Gruneisen Parameter At Elevated Temperatures

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Abstract : *Gruneisen assumed that Gruneisen constant is temperature independent. However it was observed and established that the Gruneisen constant varies with temperature. Gruneisen constant shows a drastic and dramatic change at low temperature. The variation digger from crystal to crystal in some cases there is a dip in the values of Gruneisen constant. At elevated temperatures the temperature variation of Gruneisen constant is very slight and monotonous.*

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I. Introduction

It is a well known phenomenon that the property of thermal expansion is related to anharmonic nature of atomic vibrations. If it is harmonic there will be no expansion at all. Any theory of thermal expansion and Gruneisen parameter must take into account the anharmonic vibration of atoms. Though Gruneisen considered the vibration of atoms is harmonic but brought the anharmonicity into the picture by making the frequencies of vibration volume dependent. His treatment may be considered as quasi harmonic approximation.

II. Method

The volume dependence of atomic frequency is the real conceptual, contribution of Gruneisen. Although he assumed a common constant for all modes, it was shown by many workers that there is considerable variation in the mode γ's corresponding to different modes. Much of this information has come from studies on pressure and temperature variation of Raman spectra, I.R. spectra, neutron inelastic scattering and lattice dynamics.

The average Gruneisen parameter is important as as solid state parameter. Haris and Avrami (1972) have discussed the various aspects of Physics of the Gruneisen Parameter. The data on Gruneisen parameter of crystals are too large and too scattered to be cited. Apart from the thermal Gruneisen constant, several methods of calculating Gruneisen constant have evolved. Slater (1939) showed that Gruneisen constant can be calculated from the pressure variation of bulk modulus.

$\gamma = -\left(\frac{1}{6}\right) + \frac{1}{2}\left(\frac{dB}{dP}\right)$

This is known as Slater formula Dugdale and Mc Donald (1953) modified this relation to

$$\gamma = -\left(\frac{1}{2}\right) + + \frac{1}{2}\left(\frac{dB}{dP}\right)$$

Knopoff and Shapiro (1969) showed that the pressure variation of shear modulus is important and following relation.

$\boldsymbol{\gamma} = -\left(\frac{1}{6}\right) + 0.024\left(\frac{dB}{dP}\right)\frac{dB}{dP} + 0.743\left(\frac{dG}{dP}\right)$

Where G is the shear modulus, In recent years the melting of crystals under high pressure has been studied. Knopoff and Shapiro (1969) show that the Gruneisen constant can be estimated from the pressure variation of melting temperature from the relation

$$\gamma = \frac{1}{3} - \left(\frac{1}{2}\right)\left(\frac{dlogT_m}{dlogV}\right)$$

Slater also showed that Gruneisen constant can be calculated from inter atomic potential of a crystal and used this method to evaluate Gruneisen constants of several metals from Morse potential, and several alkali halides from the Born potential. Sirdeshmukh and Rao (1972, 1975) used this method to calculate the Gruneisen constant of CaF_2 type crystals and some oxides respectively.

In recent years , considerable amount of data has been generated on Second order elastic constant (SOEC) , their pressure derivatives and third order elastic constant (TOEC). Burger (1965) and Mason(1965)

developed expression for the estimation of mode gammas and average gamma from SOEC and TOEC byt their method has not received sufficient attention. A modified method fpr evaluation of average Gruneisen constant fromfrom TOEC was proposed by Ramji Rao (1974) ; this method also has remained practically unexplored. It is also possible to estimate the Gruneisen constant from the pressure variation of Debye temperatures (Kumari and Das 1986) but data on pressure variation of Debye temperatures are not available.

III. Result And Discussion

Gruneisen assumed that Gruneisen constant is temperature independent. However it was observed and established that the Gruneisen constant varies with temperature. Gruneisen constant shows a drastic dramatic change at low temperature. The variation digger from crystal to crystal in some cases there is a dip in the values of Gruneisen constant.

At elevated temperatures the temperature variation of Gruneisen constant very slight and monotonous. After the the measurement of thermal expansion of a large number of alkali halides, Rapp and Merchant (1973) found that γ the Gruneisen constant increases lowly with temperatures. Steinberg (1981) analyzed that for twenty one metals at high temperature concluded that Gruneisen constant is independent of temperature from 300 K to substantial fraction of the melt temperatures. Slack and Huseby (1982) studied the thermal expansion of number phenacite type compounds and found that Gruneisen constant is nearly independent of temperature at high temperatures.

The general observation is that at elevated temperatures the Gruneisen constant is either independent of temperature or increases very slightly with temperatures. In case of the crystals with fluorite structures very little information is available regarding the temperature variation of Gruneisen constant at elevated temperatures. Sharma (1950) observed that the Gruneisen constant CaF_2 increases with temperature. However, Ho and Ruoff (1967) that the Gruneisen constant decreases increasing temperature over the range of 100 – 300 K. it may be mentioned that Sharma calculated the Gruneisen constant from thermal expansion data usin consant value for the bulk modulus. On the otherhand, Ho and Ruoff (1967) made their calculations on the basis of pressure variation of elastic constants. Momin and Karkhanaala (1978) studied thermal expansion of two related crystals UO_2 and ThO_2 Gruneisen constant at high temperatures and also calculated the Gruneisen constant. In case of UO_2 they observed a slight increase in the Gruneisen constant, whereas a decrease was observed in case of ThO_2. There is no clear trend regarding the temperature variation of fluorite crystals at elevated temperatures.

As such the calculation of the thermal Gruneisen constant for five fluorite type crystals has been under taken using the following equation

$$\gamma = {}^{3\alpha\, V}/_{\Psi C_V}$$

Where $\boldsymbol{\alpha}$ is the thermal expansion coefficient, V is the volume, $\boldsymbol{\Psi}$ is the compressibility and C_V is the specific heat at constant volume. For these calculations the volume has been calculated from the lattice constant data obtained in this work. The thermal expansion data is also from the present work. Data on the bulk modulus at various temperature have been calculated from from temperature derivatives of the elastic constant provide by Altrovitz and Garlich (1968, 1970, 1971) for CaF_2, SrF_2 and CdF_2 respectively. Whereas for PbF and BaF_2, data is given by Manasreh and Pederson (1984 and 1985). The specific heat C_V is calculated from the Debye temperature given by Dandekar et al (1979). PbF_2 and other crystals data was obtained from Hayes (1974).

The results are given in table (1) and also it is shown in figure (2). It may be seen that there is a systematic decrease in the value of Gruneisen constant (γ) with increasing temperature. The decrease is of the order of 10-15% over the range of 300-700 K. combining these results with the observation made by Ho and Ruoff (1967) and Momin Karkhanawala (1978), it may be concluded that in the family of crystals with fluorite structures the Gruneisen constant (γ) shows a decrease, though slight, with increasing temperatures at elevated temperatures.

In this respect, as a group, these crystals appear crystals appear to behave differently from other groups like the alkali halides. The exact reason is not clear at this moment.

Table (1): Gruneisen parameters of CaF_2 type crystals at elevated

		$\gamma_{thermal}$				
S.No	Temp. (K)	CaF_2	SrF_2	BaF_2	CdF_2	PbF_2
1	300	1.74	1.63	1.66	2.30	2.08
2	350	1.67	1.59	1.64	2.25	2.05
3	400	1.63	1.56	1.63	2.20	2.01
4	450	1.60	1.54	1.62	2.16	1.98
5	500	1.57	1.53	1.61	2.14	1.95
6	550	1.55	1.52	1.59	2.11	1.92
7	600	1.53	1.51	1.57	2.09	1.90
8	650	1.48	1.51	1.56	2.08	1.87
9	700	1.49	1.50	1.55	2.04	1.85

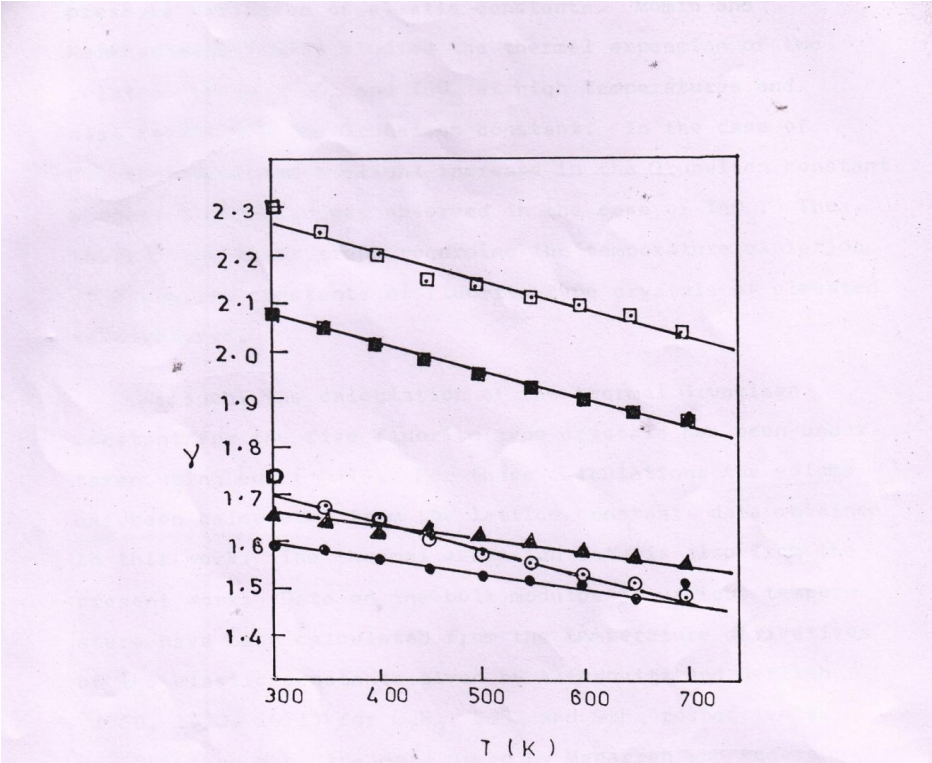

Fig. Gruneisen parameters of
⊙ - CaF_2 , ● - SrF_2 , ▲ - BaF_2
⊡ - CdF_2 , ■ - PbF_2

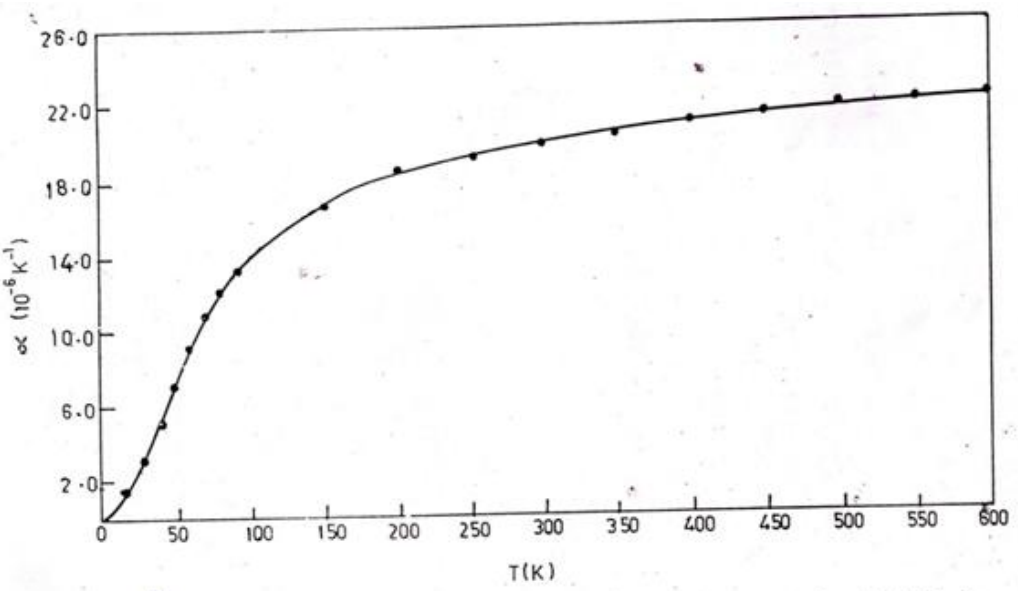

Fig. Thermal expansion of a hypothetical cubic AB_2 type crystal calculated from eq. with assumed parameters $\theta = 300K$ $Q = 3 \times 10^5$ and $\gamma = 1{\cdot}33$

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