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Ramji Rao's method of evaluating Gruneisen parameter from third order elatic constant..

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Abstract: *Thermal expansion is dirctlyn related to anharmonicity of atomic vibration. In theory of thermal expansion coefficient of solid must take into account the anharmonic nature of the lattice. Gruneisen considered the frequencies of vibration as volume dependent. his treatment is considered as quasi harmonic approximation. The volume dependence of atomic frequency is real conceptual contribution of Gruneisen.*
Our basic objective is to evaluate Gruneisen constant using third order elastic constant by Ramji Rao's method.

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I. Introduction

In recent years considerable amount of data has been generated on Second and Third order elastic constants. Though Burger and Mason developed expressions for mode gammas and average gamma for SOEC and TOEC but their methods has not recived sufficient attention. A modified method for evaluation of average gruneisen constant from Third Order elastic constant was proposed by Ramji Rao (1974) ; this method also has remained practically un explored.

Ramji Rao Mthod of Evaluating Gruneisen Constant.
The Anderson Gruneisen parameter (∂) is defined by the following equations;

$(\partial) = -(\frac{1}{\propto})(\frac{\partial lnB}{\partial T})_p$ (1)

$(\partial) = (\frac{\partial B}{\partial P}) - 1$ (2)

Where B is bulk modulus. Chang (1967)has shown that the Anderson – Gruneisen parameter ∂ is simply related to the Gruneisen parameter γ as follows ;

$\partial = 2\gamma$ (3)

Using the formalism of Ramji Rao and Srinivasan (1969), RamjiRao (1974)showed that the Anderson Gruneisen parameter for cubic crystal can be expressed in terms of the second order elastic constant and third order elastic constant as follows :

$\partial = -1 - (1/3)\left[\frac{[(C_{111}+6C_{112}+2C_{123})]}{(C_{11}+2C_{12})}\right]$ (4)

In view of equation (3) the Gruneisen constant can be expressed as :

$\gamma = -\text{-}(1/2) - (1/6)\left[\frac{C_{111}+2C_{123}}{C_{11}+2C_{12}}\right]$ (5)

This equation provides an alternatemethod for the evaluation of Gruneisen constant from SOEC and TOEC we shall call these values $\boldsymbol{\gamma_{RR}}$.

Ramji Rao applied this method to only one
crystal viz. MgO. As TOEC data are available for several cubic compound crystals, we have evaluated the Gruneisen constant for several crystals using
Ramji Rao's method. The input SOEC and TOEC is same as that we have used for Masor Burger method of evaluating Gruneisen constant. For convenience we have included the same data related to SOEC and TOEC in Table (1). The source of Thermal Gruneisen Constant was obtained with the help of following equation.

$$\gamma = \frac{3\propto V}{\Psi C_v} \quad (6)$$

where $\propto$ is the coefficient of expansion.
$\boldsymbol{\Psi}$ is the compressibility and $\mathbf{C_V}$ is the specific heat at constant volume.
It is also same as that of Mason Burger method.

The results of calculations are given in the Table (2).

Table (1)

Input data for calculation of γ'S **by Mason – Burger method and Ramji Rao's method**

SEOC 10^{11}dynes/cm^2 TOEC (10^{11}dynes γ_i^1

	C11	C12	C44	Ref	C111	C112	C123	C144	C166	Ref
LiF	12.46	4.24	6.49	a	-142.0	-26.40	15.86	8.50	-27.30-	g
NaF	9.71	2.43	2.80	a	-148.0	-27.00	28.00	4.60	-11.40	g
Nacl	3.87	0.97	0.97	a	-84.30	-2.40	4.60	2.90	-6.00	g
Kcl	4.83	0.54	0.66	a	-72.60	-1.80	1.10	2.30	-2.60	
Rbcl	3.65	0.61	0.48	a	-67.10	-95.00	0.50	1.10	-1.70	g
MgO	28.60	8.70	14.80	a	-489.50	3.50	11.30	6.60	-69.00	g
PbTe	10.795	0.764	1.343	b	185.00	-30.80	9.70	4.40	-9.80	g
GaSb	8.850	4.040	4.33	a	-47.50	-38.70	-4.40	5.00	-21.60	g
GaAs	11.88	5.38	5.94	a	-62.20	-47.40	-5.70	-0.20	-26.90	g
GaP	14.12	6.253	7.047	b	-73.70	-40.00	-13.10	-10.70	-23.40	g
CaF_2	16.42	4.398	3.370	c	-124.60	-30.90	-25.40	-12.40	-21.40	c
SrF_2	12.461	4.46	3.187	d	-82.10	-29.90	-11.10	-9.57	17.50	d
BaF_2	8.948	3.854	2.495	e	-58.40	-32.10	-20.60	12.01	8.90	e
PbF_2	9.637	4.663	2.104		-27.80, -23.90 -91.80	-40.50 -51.60	-20.50,----- 29.20,--28.20	1.80,3.40 , 2.80	-9.60, -7.20,- 6.50	h I j

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a) Anderson (1965)
b) Simon and wang (1971
c) Altrovitz and Gerlich (1969)
d) Altrovitz and Gerlich (1970)
e) Gerlich (1968)
f) Manasreh and Pederson (1984)
g) Shankar and Bhende (1986)
h) Ramacahndran and Srinivasan (1972) i)
i) Shankar and Singh (1984) Gupta et al (1984)

Detailed references are provided on the last page.

Table (2)

Values of Gruneisen constant caculated by Ramji Rao's method

S.No	Crystal	γ_{RR}	$\gamma_{thermal}$
1	LiF	1.64	1.99
2	NaF	2.4	1.57
3	NaCl	2.51	1.43
4	KCl	1.89	1.34
5	RbCl	2.13	1.25
6	MgO	1.42	1.53
7	PbTe	1.98	2.07
8	GaSb	1.87	0.59
9	GaAs	1.75	0.75
10	GaP	1.9	0.7
11	CaF_2	2.24	1.74
12	SrF_2	1.86	1.62
13	BaF_2	2.29	1.6
14	PbF_2	1.79	
		2.355	2.06

II. Result and Discussions

After the careful observation of the data following observations are made.

i) In Ramji Rao's method (Equation 5) provides the values of correct order.

ii) By and large, the values obtained from the equation (5) are larger than thermal values of Gruneisen constant.

iii) The difference between the values calculated from equation (5) varies from crystal to crystal but the difference in the two appear to have a typical value for a family of crystals. Thus the difference is about 30% in the crystals with Ca F_2 structure, and it is about 60% in crystals with Na Cl structure. Whereas the difference is about 100% - 200% in the crystals with Zn S structure.

iv) In case ofPbF_2 there is some difference between γ_{RR} and $\gamma_{thermal.}$ the difference between γ_{RR} and $\gamma_{thermal.}$ is not as much as that of γ_{RR} and γ_{MB}.

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