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Gruneisen Parameter From Third order Elastic Constant Using The Mason Burger Method:

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Abstract: *The temperature dependence of the second-order elastic constants and third order elastic constants of cubic crystalline materials is derived on the basis of Mason burger method. It is a known fact that when strain is applied to any crystalline material the frequencies of the mode and corresponding Gruneisen parameter changes according to the equation No 1,2 and 3. Where* γ_i^j *has been worked out for all the modes of crystalline material.*

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I. Introduction

Theory of thermal expansion was proposed by Gruneisen simultaneously with Debye theory of specific heat of solid. A detailed account of Gruneisen theory was proposed by Gruneisen himself in (1926). It is a known fact that thermal expansion is directly related to anharmonicity of atomic vibration. If the vibration are harmonic there will be no expansion at all. Any theory of thermal expansion of solid must take int account the anharmaonic nature of solid. Gruneisen considers the vibration as harmonic but brings anharmonicity into the picture by making the frequency of vibration as volume dependent.

Gruneisen Parameter from Third order elastic constants Mason - Burger method.

When a strain s_j is applied to a crystal, the frequencies change according to the equation

$$\nu_i = \nu_{i0}\left[1-\sum_{j=1}^{6}\gamma_i^j\, s_j\right] \qquad (1)$$

Where ν_{i0} a frequency of a mode in the standard state and γ_i^j is the corresponding Gruneisen parameter. A particular Gruneisen parameter is given by

$$\gamma_i^j = -\frac{\partial \nu_i / \partial s_j}{\nu_{i0}} \qquad (2)$$

Mason (1965) presented a method of obtaining the γ_i^j's. for this purpose he used general expression developed by Burger(1965) to evaluate γ_i^j from SOEC (Second Order Elastic Constant) and TOEC (Third Order Elastic Constant). General expression is

$$\gamma_i^j = \left[U_j \mathrm{U_k} + \langle\frac{N_p N_q}{2C}\rangle\left(C_{jkpq} + U_r U_S C_{jkprqs}\right)\right] \qquad (3)$$

Where the U's are direction cosines for particle displacement and N_p $and N_q$ aredirection cosines for the propagation direction. C_{jkpq} C_{jkprqs} are SOEC and TOEC in double index notation. From this, the Gruneisen parameters for specific mode and directions can be obtained. Thus for a longitudinal wave along the (100) direction, this equation gives (in single index notation)

$$: \gamma_i^1 = \frac{-\langle 3C+11\, C_{111}\rangle}{2C_{11}} \qquad (4)$$

Expressions have been worked out for all other modes and directions of propagations pertaining to γ_i^1 and are given in table (1) : other γ_i^j's are not of consequence. Mason evaluated the mode Gruneisen parameters for Si and Ge from the expressions in the table. Mason pointed out that the average (γ_{MB}) of these mode

gammas should be equal to the high temperature Gruneisen parameter obtained from thermal expansion data: fairly good agreement was obtained in the case of silicon and germanium.

Mason's calculation was confined to Si and Ge. The method has not been applied o other crystals nor has ias been critically examined otherwise. Data on third order elastic constant for several have become available recently. Shanker and Bhende (1986) have reviewed the data on TOEC of compound crystals including crystals with CaF_2 structures. Although our interestis in crystals with CaF_2 . structure, it was considered worthwhile to apply the Mason – Burger method to all compound crystals for which , data on TOEC is available and to examine the systematic. Accordingly calculations are made for seven with NaCl structures and three crystals ZnS structure and four crystals with CaF_2 structure.

Table 1

No	Type of Waves	Direction of Propagation	Direction of Polarization	Equation for γ_i^1
1	2	3	4	5
1	Long	100	100,010, 001	$\frac{3C_{11}+C_{111}}{2C_{11}}$
2	Shear	100	010, 001	$\left[\frac{C11+C116}{2C44}\right]$
3	Long	010, 001	010,001	$\left[\frac{C_{12}+C_{112}}{2C_{11}}\right]$
4	Shear	010, 001	100,100	$\left[\frac{2C_{44}+C_{12}+C_{166}}{2C_{44}}\right]$
5	Shear	010, 001	001,010	$\left[\frac{C_{12}+C_{144}}{2C_{44}}\right]$
6	Long	110, 101	110,101	$\left[\frac{2C_{12}+C_{112}+2C_{144}+C_{123}}{2(C_{11}+C_{12}+2C_{44}}\right]$
7	Shear	011, 01¯1	011¯,011	$\left[\frac{2C_{12}+C_{112}-C_{123}}{2(C_{11}-C_{12})}\right]$
8	Shear	011, 01¯1	100,100	$\left[\frac{C12 \quad +2C_{44}+C_{166}}{2C_{44}}\right]$
9	Long	110, 110, 101, 101	110,.11¯0,101,101¯	$\left[\frac{2(C_{22}+C_{12}+C_{44})+\frac{C_{111}}{2}+\frac{3}{2}C_{112}+2C_{166}}{2[C_{11}+C_{12}+2C_{44}]}\right]$
10	Shear	110, 110, 101,101	11¯ 0, 110,101¯,101	$\left[\frac{2C_{11}+\left(\frac{C_{111}-C_{112}}{2}\right)}{2(C_{11}-C_{12})}\right]$
11	Shear	110,110,101,101	001,001,010,010, ¯	$\left[\frac{C_{11}+C_{12}+(C_{144}+C_{166})}{4C_{44}}\right]$
12	Long	111, 111, 111, 111	111,11¯1,11$\bar{1}$,11¯1	$5\frac{5C_{11}+10C_{12}+8C_{44}+C_{111}+6C_{112}+2C_{123}+4C_{1448}C_{166}}{6(c_{11}+2c_{12}+4c_{44})}$
13	Shear	111,111,111,111	1¯1¯2,1¯12,1¯1¯2¯,112	$\left[\frac{4C_{11}+5C_{12}C44+\quad+\left(\frac{C_{111}+3C_{112}}{2}\right)+\frac{C_{144}+C_{166}}{2-2C_{123}}}{6(C_{11}-C_{12}+C44\ )}\right]$
14	Shear	111,11¯1,111,111	1¯10.110,1¯10,110	$\left[\frac{2C_{11}+C_{12}+C_{44}+\frac{(C_{6666}-C_{666})+(C_{1122}+C_{166})/2}{2}}{2(C_{11}-C_{12}-C_{44})}\right]$

Table (2) Input data for calculation of γ'S by Mason – Burger method γ_i^1

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

	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

References

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) Shankar and Singh (1984)Gupta et al . (1984)

Detailed references are provided on the last page

Table 3

γ's for some crystals with NaCl Structure

	Column2	**Column3**	**Column4**	**Column5**	**Column6**	**Column7**	**Column8**
			γ_i^1				
i	LiF	KCl	NaCl	NaF	RbCl	MgO	PbTe
1	4.19	6.01	9.39	6.12	7.69	7.05	7.06
2	1.14	-1.68	1.09	0.3	-2.03	1.36	-0.37
3	0.89	0.19	0.52	1.26	0.16	1.5	-0.19
4	0.77	0.56	1.59	0.6	0.13	1.03	2.36
5	-0.98	-2.15	-1.99	-1.25	-1.78	-0.51	-1.92
6	-0.24	-0.32	-0.54	-0.42	0.2	0.39	-0.14
7	2.03	0.28	1.32	3.44	0.17	2.23	-0.73
8	0.77	0.56	1.59	0.6	0.13	1.03	2.36
9	2	2.46	3.68	3.02	2.88	3.14	2.84
10	2	2.96	5.5	2.82	4.16	3.51	3.62
11	0.08	-1.92	0.44	-0.47	-1.9	0.42	-1.14
12	1.05	1.2	1.8	1.49	1.42	1.92	1.61
13	1.45	0.83	2.2	2.36	1.08	1.95	0.61
14	1.07	2.46	4.07	1.94	3.48	2.12	3.52

Table 4 Mode γ,s for some crystals with ZnS Structure

$$\gamma_i^1$$

i	Ga Sb	GaAs	Ga P
1	1.18	1.11	1.1
2	1.47	1.36	0.65
3	1.51	1.42	1.45
4	1.02	0.95	0.21
5	-1.04	-0.5	0.31
6	0.39	0.58	1
7	1.9	1.71	1.38
8	1.02	0.95	0.21
9	1.82	1.72	1.44
10	0.97	-0.92	-0.95
11	0.21	0.42	0.48
12	1.33	1.35	1.29
13	0.96	0.9	0.56
14	-0.51	-0.39	0.38

Table (5) γ's for some crystals with CaF_2 structure

$$\gamma_i^1$$

	CaF2	SrF2	BaF2	PbF2		
				Ref h	Ref i	Ref j
1	2029	1.79	1.76	-0.05	-0.2205	0.149
2	0.738	0.79	0.009	0.008	-0.5095	-0.745
3	1.08	1.06	1.45	1.42	10932	2.435
4	1.52	1.04	0.001	0.17	-0.333	-0.563
5	1.18	0.79	1.65	-0.53	-1.857	-1.77
6	1.477	1.26	1.88	1.07	1.507	2.255
7	0.241	0.24	0.15	0.22	0.253	1.414
8	1.52	1.04	0.01	0.17	-0.333	-0.563
9	2.11	1.76	1.72	1.3	1.544	1.985
10	0.39	0.423	-0.35	-2.15	-2.73	-2.254
11	0.96	0.79	0.82	-0.77	-1.183	-1.259
12	2.08	1.7	1.84	1.33	1.666	1.99
13	4.35	0.36	0.07	-0.46	-0.73	-0.287
14	0.604	0.29	0.03	-0.171	-2.242	-2.408

Table 6 Comparison of average Gruneisen Constant from mo

	Crystal	(γ_{MB})	($\gamma_{thermal}$)
1	LiF	1.16	1.99
2	KCl	0.81	1.34
3	NaCl	2.12	1.43
4	NaF	1.55	1.57
5	RbCl	1.1	1.25
6	MgO	1.94	1.53
7	PbTe	1.3	2.07
8	GaSb	0.73	0.59
9	GaAs	0.76	0.75
10	GaP	0.63	0.7
11	CaF2	1.46	1.74
12	SrF_2	0.92	1.62
13	BaF_2	0.79	1.6
14	PbF_2	-0.07	---
		-2.23	2.06
		0.027	

de gamma($\gamma_{MB)}$ and thermal gamma ($\gamma_{thermal}$)

II. Result And Discussion

The input data for the evaluation of the mode gammas is given in table (2). The values of mode for the three structures group is studied and given in the table (3), (4) and (5)from careful examination following trends can be noticed.

i) The magnitude of γ_i's (the upper index is dropped) varies over a wide range taking values as large as 9.
ii) The mode γ's have both +ve and –ve signs.
iii) For a crystal, different mode γ's take +ve and –ve signs.
iv) A given γ_i may have +ve and –ve values in different crystals.
v) As far as the signs of individual γ_i's are concerned there is no rigid structure dependence. Yet some trends do appear. Thus in crystals with NaCl structure γ_5, γ_6 and γ_{11} tend to have –ve , where as in ZnS structere, γ_5 and , γ_{14} *show this trend to be* $-ve$. in CaF_2 structure all γ_i tend to be +ve
vi) , γ_1 and γ_4, γ_8, γ, γ_9, $\gamma_{12}$and γ_{13}

Are uniformly +ve in crystals for which calculations have been made. the fact that γ_i is always a positive taken together with equation (28), leads to the empirical condition.

$$\mathbf{3}\,\boldsymbol{C_{11}} < |\boldsymbol{C_{111}}|$$

For cubic crystals . this relation may be useful in checking the values of $C_{111.}$

In case of PbF_2 , the experimental values of TOEC are not available. However, in view of interest in PbF_2 several lattice dynamical studies have been carried out and TOEC are available from three different models. Ramacahandran and Srinivasan (1972) calculated the TOEC from the shell model . Shankar and Singh (1989) used the method of finite deformation and calculated the TOEC using the catlow–type potential. Gupta et al

(1986) pointed out deficiencies in the model adopted by Shankar and singh. They employed a more refined model including additional interaction.TOEC from these three models are given in table (2). It may be seen that there is considerable difference in three set of TOEC. We have used all the three set of sets to calculate mode gammas as well as average γ_{MB}. The mode gammas canot provide much information about the relative merit of the model used. However, the values of γ_i show s strong variation. The empirical condition printed abov ($3\ C_{11} < |C_{111)}|$) is satisfied only by the values of TOEC obtained by Gupta et al.

vii) The average value of γ_{MB} calculated for the mode gammas agrees reasonably with $\gamma_{thermal.}$ The agreement is with in 30-50%in the crystals with Na Cl structure and 10-% 20% with crystals with ZnS structure and 30 to 80% in crystals with CaF_2 structure. The agreement is very less in case of PbF_2. In fact with two sets of TOEC a –ve value is is obtained for γ_{MB}. A positive value is obtained only with set given by Gupta et al.

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