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Higher Order Elastic Constants, Gruneisen Parameters and Lattice Thermal Expansion of Trigonal Calcite

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Abstract: The second- and third-order elastic constants of trigonal calcite have been obtained using the deformation theory. The strain energy density derived using the deformation theory is compared with the strain dependent lattice energy obtained from the elastic continuum model approximation to get the expressions for the second- and third-order elastic constants. Higher order elastic constants are a measure of the anharmonicity of a crystal lattice. The seven second-order elastic constants and the fourteen non-vanishing third-order elastic constants of trigonal calcite are obtained. The second-order elastic constants C_{11} , which corresponds to the elastic stiffness along the basal plane of the crystal is greater than C_{33} , which corresponds to the elastic stiffness tensor component along the c-axis of the crystal. First order pressure derivatives of the second-order elastic constants of calcite are evaluated. The higher order elastic constants are used to find the generalized Gruneisen parameters of the elastic waves propagating in different directions in calcite. The Brugger gammas are evaluated and the low temperature limit of the Gruneisen gamma is obtained. The results are compared with available reported values.

Key words: Elastic properties; Thermal expansion; Acoustical properties

Introduction

Knowledge of higher order elastic constants is essential for the study of the anharmonic properties of solids. Elastic constants also provide insight in to the nature of binding forces between the atoms since they are represented by the derivatives of the internal energy. A complete set of elastic constants for materials is essential to estimate physical parameters such as Debye temperature, compressibility and acoustic anisotropy.

There are more than ten compounds that crystallize with calcite (CaCO_3) structure at ambient conditions. The calcite-structure carbonates (space group $R\bar{3}C$) represent a mineral group that is structurally simple and different from oxides and silicates; the slightly distorted octahedra are exclusively corner-linked through shared oxygen anions of CO_3 groups. In the calcite there are six different ion-pair types, but the carbon atoms are deeply buried inside oxygen triads so the carbon atoms will not be considered explicitly and the number of different ion-pairs is reduced to three: metal-ion-metal-ion (M-M), metal-ion-oxygen-ion (M-O) and oxygen-ion-oxygen-ion (O-O).¹ The trigonal class of crystals has seven second-order elastic constants and fourteen third-order elastic constants. Thermal expansion and elastic properties of single crystal calcite are extensively studied using ultrasonic techniques²⁻⁵ using Brillouin spectroscopy⁶ and using other techniques.⁷⁻¹²

In the present study we make an attempt to calculate the complete set of second and third-order elastic constants, pressure derivatives of the second-order elastic constants, generalized Gruneisen parameters of elastic waves and low temperature thermal expansion of trigonal calcite and are compared with those obtained by other workers.^{2,4-6,10-12}

Higher order elastic constants of calcite.

Considering interactions up to third nearest neighbours in calcite, the potential energy per unit cell¹³ is

$$\phi = \phi_0 + \sum_{I=1}^3 \phi R(I) + \sum_{J=1}^3 \phi R(J) \quad (1)$$

The components of the interatomic vectors under a homogeneous deformation are given by $R'_i(I) = R_i(I) + \sum_j \epsilon_{ij} R_j(I)$ and $R'_i(J) = R_i(J) + \sum_j \epsilon_{ij} R_j(J) + W_i$ (2)

Where ϵ_{ij} the deformation parameters and are related to the macroscopic Lagrangian strains η_{ij} by

$$\eta_{ij} = \frac{1}{2} \left[\epsilon_{ij} + \epsilon_{ji} + \sum_k \epsilon_{ki} \epsilon_{kj} \right] \quad (3)$$

W_i are the components of the internal displacements of the lattice of particles of type J relative to the lattice of particles of the type I and are replaced by the relative internal displacement

$$\bar{W}_i = W_i + \sum_j \epsilon_{ij} W_j \quad (4)$$

It is to be noted that inversion symmetry holds good lattice dynamically within a good approximation. Hence when the crystal is homogeneously deformed¹⁴ equation (2) becomes

$$R'_i(J) = R_i(J) + \sum_j \epsilon_{ij} R_j(J) \quad (5)$$

We expand the potential energy of the crystal in powers of the changes in the scalar products of the interatomic vectors¹⁵ and incorporate the two and three-body interactions in the expression for the potential energy. For instance, the two-body and three-body potentials among the first neighbour atoms (I atoms) are written, respectively, as

$$\phi^{(2)} = \frac{1}{2} \sum_I \left\{ \frac{1}{2} \alpha_1 [R'(I) \cdot R'(I) - R(I) \cdot R(I)]^2 + \frac{1}{6} \xi_1 [R'(I) \cdot R'(I) - R(I) \cdot R(I)]^3 \right\}$$

and

$$\phi^{(3)} = \frac{1}{2} \sum_I \left[\frac{1}{2} \sigma_1 \left\{ [R'(I).R'(I') - R(I).R(I')]^2 + [R'(I).R'(I'') - R(I).R(I'')]^2 \right\} \right. \\ \left. + \frac{1}{6} v_1 \left\{ [R'(I).R'(I') - R(I).R(I')]^3 + [R'(I).R'(I'') - R(I).R(I'')]^3 \right\} \right] \quad (6)$$

Here I' and I'' are the neighbouring atoms lying on either side of a given atom I . The second-order parameters for the two-body interactions as well as the three-body interactions for the first neighbour atoms (I atoms) are written, respectively as α_1 and σ_1 . The third-order parameters for the two-body interactions as well as the three-body interactions for the first neighbour atoms (I atoms) are written, respectively as ξ_1 and v_1 .

The strain energy derived from continuum model approximation¹⁴ is

$$U = \frac{1}{2!} \sum_{ijkl} C_{ijkl} \eta_{ij} \eta_{kl} + \frac{1}{3!} \sum_{ijklmn} C_{ijklmn} \eta_{ij} \eta_{kl} \eta_{mn} + \dots \quad (7)$$

where C_{ijkl} and C_{ijklmn} are the second and third order elastic constants in tensor form respectively. Comparing this with the lattice energy from equation (6) we get the expressions for the second-order and third-order elastic coefficients of trigonal calcium carbonate.

The second-order elastic coefficients are given in Voigt notation in equation (8)

$$C_{11} = [14.06\alpha_1 + 1.56\alpha_2 + 25.00\alpha_3 + 7.03\sigma_1 + 0.78\sigma_2]B \quad (8a)$$

$$C_{12} = [4.69\alpha_1 + 0.52\alpha_2 + 8.33\alpha_3 - 2.34\sigma_1 - 0.26\sigma_2]B \quad (8b)$$

$$C_{13} = [0.69\alpha_2 + 2.78\alpha_3 - 0.35\sigma_2]P^2 B \quad (8c)$$

$$C_{14} = [-0.60\alpha_2 - 4.81\alpha_3 + 0.30\sigma_2]PB \quad (8d)$$

$$C_{33} = [0.46\alpha_2 + 0.46\alpha_3 + 0.46\sigma_2]P^4 B \quad (8e)$$

$$C_{44} = [0.69\alpha_2 + 2.78\alpha_3 + 0.35\sigma_2]P^2 B \quad (8f)$$

$$C_{66} = [4.69\alpha_1 + 0.52\alpha_2 + 8.33\alpha_3 + 4.69\sigma_1 + 0.52\sigma_2]B \quad (8g)$$

where $B = 10^{-2}a^4$

Here 'a' is the lattice parameter and 'P' is the axial ratio c/a of the trigonal crystal calcite. The second-order parameters characterizing the two-body interactions α_1 , α_2 and α_3 for the first, second and third neighbours and the three-body interactions σ_1 and σ_2 for the first and second neighbours have been obtained by substituting the values of C_{ij} measured by Chen et al⁶ and are given in **Table I**. These values are used in equation (8) to obtain the second-order elastic constants of calcite. The values of second-order elastic constants of calcite thus obtained are given in **Table 2** along with other reported values of Dandeker², Hearmon⁴, Thanh and Lacam⁵, Chen et al⁶ and Pavese et al.¹⁰

Table 1 Values of second-order potential parameters (in G Pa) of Calcite.

Parameters	Values
$\alpha_1 B$	10.15
$\alpha_2 B$	3.18
$\alpha_3 B$	0.55
$\sigma_1 B$	-1.47
$\sigma_2 B$	-2.38

Table 2 Second-order elastic constants of Calcite (in G Pa) along with the reported values

C_{ij}	Present Values	Reported Values				
		Ref. [2]	Ref. [4]	Ref. [5]	Ref. [6]	Ref. [10]
C_{11}	149.4	148.0	144.0	145.7	149.4	153.0
C_{12}	57.9	55.4	53.9	55.9	57.9	55.0
C_{13}	53.5	54.5	51.1	53.5	53.5	50.0
C_{14}	-18.1	-20.8	-20.5	-20.5	-20.0	13.0
C_{33}	85.2	85.7	84.0	85.3	85.2	82.0
C_{44}	34.1	32.8	33.5	33.4	34.1	37.0
C_{66}	45.7	--	--	--	--	37.0

The third-order elastic coefficients are given in Voigt notation in equation (9).

$$C_{111} = [32.23\xi_1 + 0.98\xi_2 + 62.50\xi_3 + 7.32v_1 - 0.49v_2]D \quad (9a)$$

$$C_{112} = [2.93\xi_1 + 0.33\xi_2 + 20.82\xi_3 + 1.46v_1 + 0.16v_2]D \quad (9b)$$

$$C_{113} = [0.43\xi_2 + 6.95\xi_3 + 0.22v_2]P^2 D \quad (9c)$$

$$C_{114} = [-0.38\xi_2 - 12.02\xi_3 - 0.19v_2]PD \quad (9d)$$

$$C_{123} = [0.14\xi_2 + 2.31\xi_3 - 0.07v_2]P^2 D \quad (9e)$$

$$C_{124} = [-0.13\xi_2 - 4.01\xi_3 + 0.06v_2]PD \quad (9f)$$

$$C_{133} = [2.26\xi_2 + 9.03\xi_3 - 1.13v_2]P^2 D \quad (9g)$$

$$C_{134} = [-0.17\xi_2 - 1.34\xi_3 + 0.08v_2]P^3 D \quad (9h)$$

$$C_{144} = [0.14\xi_2 + 2.31\xi_3 - 0.07v_2]P^2 D \quad (9i)$$

$$C_{155} = [0.43\xi_2 + 6.95\xi_3 - 0.07v_2]P^2 D \quad (9j)$$

$$C_{222} = [26.36\xi_1 + 1.19\xi_2 + 76.27\xi_3 + 13.18v_1 - 0.27v_2]D \quad (9k)$$

$$C_{333} = [0.13\xi_2 + 0.13\xi_3 + 0.13v_2]P^6 D \quad (9l)$$

$$C_{344} = [0.19\xi_2 + 0.77\xi_3 + 0.10v_2]P^4 D \quad (9m)$$

$$C_{444} = [0.17\xi_2 + 1.34\xi_3 + 0.04v_2]P^3 D \quad (9n)$$

where $D = 10^{-3}a^6$

The third-order potential parameters characterizing the two-body interactions ξ_1 , ξ_2 and ξ_3 for the first, second and third neighbours and the three-body interactions v_1 and v_2 for the first and second neighbours have been obtained substituting the values of C_{ijkl} reported by Kaga¹¹ in equation (9). The values of the third-order potential parameters thus calculated are given in **Table 3**. The values from **Table 3** have been used in equation (9) to obtain all the third-order elastic constants of calcite. The values of third-order elastic constants thus obtained for calcite are collected in **Table 4** along with the reported values of Kaga.¹¹

Table 3 Values of third-order potential parameters (in G Pa) of Calcite

Parameters	Values
$\xi_1 D$	-8.61
$\xi_2 D$	1.09
$\xi_3 D$	-2.65
$v_1 D$	-18.80
$v_2 D$	-0.87

Pressure derivatives of the second-order elastic constants

The stress tensor τ_{ij} is defined by Murunaghan¹⁶ as

$$\tau_{ij} = \frac{\rho}{\rho_0} \sum_{pq} \left[\frac{\delta x_i}{\delta a_p} \right] \left[\frac{\delta U}{\delta_{pq}} \right] \left[\frac{\delta x_j}{\delta a_q} \right] \quad (10)$$

where ρ and ρ_0 are the densities a_j and x_j are the co-ordinates of material particles in the natural and deformed state respectively. η_{ij} is the Lagrangian strain parameter and U is the strain energy density.

Comparing this with the expression for stress

$$\tau_{ij} = -p\delta_{ij} + \sum_{kl} C'_{ijkl} \beta_{kl} \quad (11)$$

β_{kl} , being the infinitesimal strain parameter and p being the pressure, the expressions for the effective second-order elastic constants C'_{ijkl} can be obtained to the first order in strains¹¹, ϵ_{11} and ϵ_{33} as

$$\begin{aligned} C'_{11} &= C_{11} + \epsilon_{11} [C_{111} + C_{112} + 3C_{11} + C_{12}] + \epsilon_{33} [C_{113} + C_{13}] \\ C'_{12} &= C_{12} + \epsilon_{11} [C_{111} + 2C_{112} - C_{222} + 2C_{12}] + \epsilon_{33} [C_{123}] \\ C'_{13} &= C_{13} + \epsilon_{11} [C_{113} + C_{123} + C_{13}] + \epsilon_{33} [C_{133} + C_{13}] \\ C'_{14} &= C_{14} + \epsilon_{11} [C_{114} + C_{124} + 2C_{14}] + \epsilon_{33} [C_{134}] \\ C'_{33} &= C_{33} + \epsilon_{11} [2C_{133} + 2C_{13}] + \epsilon_{33} [C_{333} + 3C_{33}] \\ C'_{44} &= C_{44} + \epsilon_{11} [C_{144} + C_{155} + C_{44}] + \epsilon_{33} [C_{344} + C_{44}] \\ C'_{66} &= C_{66} + \epsilon_{11} \left[\frac{1}{2} [C_{222} - C_{112}] + 2C_{66} \right] + \epsilon_{33} \left[\frac{1}{2} [C_{113} - C_{123}] \right] \end{aligned} \quad (12)$$

$$\text{where } \epsilon_{11} = \frac{[C_{13} - C_{33}]p}{[C_{11} + C_{12}]C_{33} - 2C_{13}^2} \text{ and } \epsilon_{33} = \frac{[2C_{13} - C_{11} - C_{12}]p}{[C_{11} + C_{12}]C_{33} - 2C_{13}^2}$$

The values of second-order and third-order elastic constants of calcite, given in **Table 2** and **Table 4** respectively, are substituted in equation (12) to get the pressure derivatives of the second-order elastic constants of calcite. The values thus obtained are given in **Table 5** along with the reported values of Kaga¹¹ and Ramji Rao and Padmaja.¹²

Table 4. Thirdorder-elastic constants of calcite (in G Pa) along with the reported values

C_{ijk}	Present work	Reported values [11]
C_{111}	-579	-579
C_{112}	-108	-147
C_{113}	-211	-193
C_{114}	108	218
C_{123}	-69	-41
C_{124}	36	10
C_{133}	-239	-239
C_{134}	131	82
C_{144}	-69	-69
C_{155}	-209	-139
C_{222}	-675	-675
C_{333}	-498	-498
C_{344}	-262	-195
C_{444}	-135	33

Table 5 Pressure derivatives of the second order elastic constants of calcite

dC'_{ij} / dp	Present work	Reported values	
		Ref [11]	Ref [12]
dC'_{11} / dp	1.80	3.02	2.00
dC'_{12} / dp	0.59	2.05	1.04
dC'_{13} / dp	2.16	3.19	2.19
dC'_{14} / dp	-1.39	-1.25	-1.26
dC'_{33} / dp	3.02	2.80	1.82
dC'_{44} / dp	2.56	0.92	0.92
dC'_{66} / dp	1.11	0.49	0.48

Generalized Gruneisen parameters of elastic waves and low temperature thermal expansion

Uniaxial crystals are characterized by two principal linear expansion coefficients, $\alpha_{//}$, parallel to the unique axis and α_{\perp} , perpendicular to the unique axis. The behavior of these expansion coefficients at low temperature is governed by two generalized Gruneisen parameters $\gamma_j(\theta, \phi)$, defined as

$$\gamma'_j(\theta, \phi) = -\frac{1}{v_j(\theta, \phi)} \frac{\partial v_j(\theta, \phi)}{\partial \epsilon'} \quad \text{and} \quad \gamma''_j(\theta, \phi) = -\frac{1}{v_j(\theta, \phi)} \frac{\partial v_j(\theta, \phi)}{\partial \epsilon''} \quad (13)$$

where $v_j(\theta, \phi)$, is the velocity of the elastic waves traveling in a direction (θ, ϕ) , j , is the polarization index of the wave, θ , is the angle the direction of wave propagation makes with the unique axis, ϕ , is the azimuthal angle ϵ' is a uniform areal strain perpendicular to the unique axis and ϵ'' is a uniform longitudinal strain parallel to the unique axis. These generalized Gruneisen parameters can be calculated from the second and third-order elastic constants of a solid as shown by Ramji Rao and Srinivasan¹⁷. Using the second and third-order elastic constants the elastic wave velocities $v_j(\theta, \phi)$, the generalized Gruneisen parameters $\gamma'_j(\theta, \phi)$ and $\gamma''_j(\theta, \phi)$ for different values of θ and ϕ at intervals of 5° ranging from 0 to 90° are calculated.

The linear thermal expansion coefficients of a uniaxial crystal are given by

$$V\alpha_{//} = [2S_{13}\gamma'(T) + S_{33}\gamma''(T)]C_v(T) \quad \text{and} \\ V\alpha_{\perp} = [(S_{11} + S_{12})\gamma'(T) + S_{13}\gamma''(T)]C_v(T) \quad (14)$$

Here V is the molar volume, the S_{ij} are the elastic compliance coefficients, and $C_v(T)$ is the molar specific heat at temperature T . $\gamma'(T)$ and $\gamma''(T)$ are the effective Gruneisen functions, being the weighted averages of the Gruneisen functions of all the normal modes of the crystal. At very low temperatures, the effective Gruneisen parameters are determined by the mode gammas of the elastic waves and $\gamma'(T)$ and $\gamma''(T)$ attain limiting values, γ'_0 and γ''_0 . In terms of $v_j(\theta, \phi)$, $\gamma'_j(\theta, \phi)$ and $\gamma''_j(\theta, \phi)$, these limits are defined by

$$\gamma'_0 = \frac{\sum_{j=1}^3 \int v_j^{-3}(\theta, \phi) \gamma'_j(\theta, \phi) d\Omega}{\sum_{j=1}^3 \int v_j^{-3}(\theta, \phi) d\Omega} \quad \text{and} \quad \gamma''_0 = \frac{\sum_{j=1}^3 \int v_j^{-3}(\theta, \phi) \gamma''_j(\theta, \phi) d\Omega}{\sum_{j=1}^3 \int v_j^{-3}(\theta, \phi) d\Omega} \quad (15)$$

The integration is over the entire solid angle. We have obtained the values of γ'_0 and γ''_0 by numerical integration over the solid angle. The integrals are evaluated by dividing θ and ϕ into intervals of 5° and the values are obtained. Brugger and Fritz¹⁸ have defined the functions $\gamma_{\perp}^{Br} = V\alpha_{\perp} / C_v \chi_{iso}$ and $\gamma_{//}^{Br} = V\alpha_{//} / C_v \chi_{iso}$ where χ_{iso} is the isothermal compressibility. Combining equation (14) and equation (15) the low temperature limits of the Brugger gammas are given by

$$\gamma_{\perp}^{Br}(0) = [(S_{11} + S_{12})\gamma'_0 + S_{13}\gamma''_0] / \chi_{iso} \quad \text{and} \quad \gamma_{//}^{Br}(0) = [2S_{13}\gamma'_0 + S_{33}\gamma''_0] / \chi_{iso} \quad (16)$$

Here S_{ij} are the elastic compliance coefficients and

$$\chi_{iso} = 2[S_{11} + S_{12} + S_{13}] + 2S_{13} + S_{33}$$

Using the values of γ'_0 and γ''_0 we get $\gamma_{\perp}^{Br}(0)$ and $\gamma_{\parallel}^{Br}(0)$. Using these two values, the low temperature limit γ_L can be calculated using the formula

$$\gamma_L = 2\gamma_{\perp}^{Br}(0) + \gamma_{\parallel}^{Br}(0) \tag{17}$$

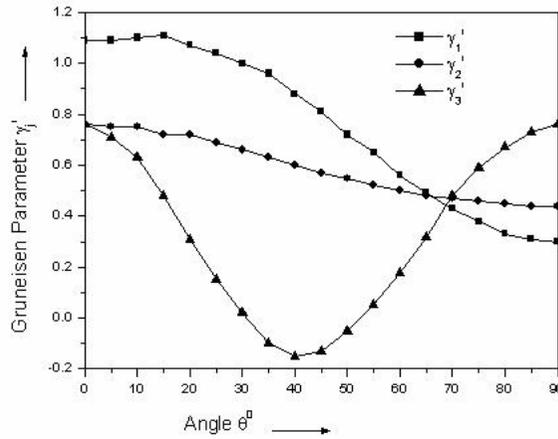


Figure 1: Variation of the generalized GP's γ'_j with angle θ for the different acoustic waves in calcite

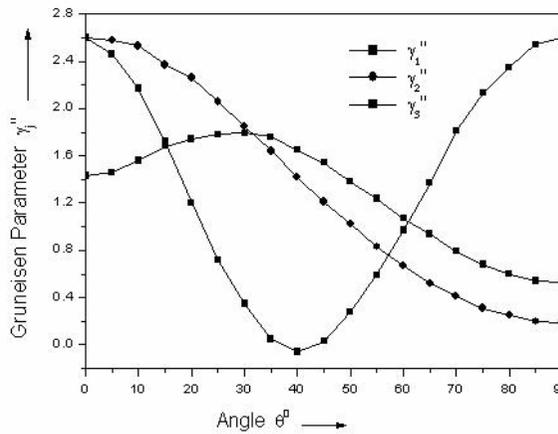


Figure 2 Variation of the generalized GP's γ''_j with angle θ for the different acoustic waves in calcite.

Figure 1 and **Figure 2** show the variations of generalized Gruneisen parameters γ' and γ'' for the three elastic waves as a function of θ . We have calculated the values of γ'_0 and γ''_0 using equation (14) as $\gamma'_0 = 0.41$ and $\gamma''_0 = 1.14$. Using these values in equation (15) the Brugger gammas are calculated. The values are $\gamma_{\perp}^{Br}(0) = -0.16$ and $\gamma_{\parallel}^{Br}(0) = 1.17$. The low temperature limit of the Gruneisen gamma is obtained as $\gamma_L = 0.85$ for calcite.

Conclusion

Calcite possesses seven second-order elastic constants. The values of second-order elastic constants of calcite obtained in the present work are collected in **Table 2** along with the reported values of Dandekar², Hearmon⁴, Vo Thanh and Lacam⁵, Chen et al⁶ and Pavese et al¹⁰. The elastic constant C_{33} , which corresponds to the wave propagation along the c- axis of the crystal, is in reasonable agreement with the available experimental values. Also it is found that C_{33} is less than C_{11} , which corresponds to the binding forces along the basal plane of the crystal. Therefore, in calcite the bonding between the atoms along the a-b plane is stronger than that between the atoms along the c-direction. Measurements of elastic constants except that along the crystallographic axes may lead to imprecise results due to the uncertainty in the orientation of single crystals. This may be a reason for the deviation of the present second order elastic constants from the corresponding experimental values.

Dandekar² has measured the elastic constants of calcite using ultrasonic technique. The values of C_{11} , C_{12} , C_{13} , C_{14} , C_{33} and C_{44} differ from his values by 0.9%, 4.5%, 1.8%, 13%, 0.6% and 4% respectively. The reported values of these constants, by different workers^{2,4-6,10}, differ considerably among themselves.

The third-order elastic constants evaluated in the present work are given in **Table 4** along with the reported values of Kaga¹¹. The results obtained in the present work are of the same order and are in good agreement with those of Kaga¹¹. C_{333} is smaller than C_{111} and C_{222} which means that the anisotropy along the basal plane is more pronounced than that along the c-axis. All the third-order elastic constants are negative except C_{114} , C_{124} and C_{134} for calcite.

The pressure derivatives of the second-order elastic constants of calcite obtained in the present work are given in **Table 5** along with the reported values of Kaga¹¹ and Ramji Rao and Padmaja¹². The results obtained in the present work are of the same order and in good agreement with those of the other workers^{11,12}. It is found that the pressure derivative dC'_{33}/dp is the largest, which indicates that the compressibility along the c-axis is higher than that along the other planes.

The mode Gruneisen parameters of calcite for different acoustic wave propagation directions are calculated. This data give evidence for thermal expansion anisotropy of the material for various acoustic modes. γ''_j , which corresponds to the change in frequencies due to a uniform longitudinal strain along the c axis of calcite, is found to be more anisotropic than γ'_j , which refers to change in frequencies due to a uniform areal strain perpendicular to the c-axis. Hence the vibrational anharmonicity along the c-axis is more pronounced than that along the a-b plane in calcite. The variations of γ'_j and γ''_j with θ are shown in **Figure 1** and **Figure 2**. The anisotropy in all the graphs of γ'_j and γ''_j vs. θ accounts for the pronounced anharmonicity of the solid in certain specific directions. The average Gruneisen function are $\gamma_{\perp}^{Br}(0) = -0.16$ and $\gamma_{\parallel}^{Br}(0) = 1.17$. This suggests that the anisotropy in the thermal expansion along the a-b plane is more pronounced than that

along the c-axis. The low temperature limit of the lattice thermal expansion γ_L is calculated from mode Gruneisen gammas and is found to have a value $\gamma_L = 0.85$. The low temperature limit γ_L is positive and hence we expect the volume lattice thermal expansion to be positive down to 0 K for calcite.

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