

Effective secondorder elastic constants of a strained crystal using the finite strain elasticity theory

R. Ramji Rao and A. Padmaja

Citation: [Journal of Applied Physics](#) **62**, 440 (1987); doi: 10.1063/1.339818

View online: <http://dx.doi.org/10.1063/1.339818>

View Table of Contents: <http://scitation.aip.org/content/aip/journal/jap/62/2?ver=pdfcov>

Published by the [AIP Publishing](#)

Articles you may be interested in

[Second-order elastic constants of pentaerythritol tetranitrate and cyclotrimethylene trinitramine using impulsive stimulated thermal scattering](#)

[J. Appl. Phys.](#) **104**, 073517 (2008); 10.1063/1.2981044

[Second-order elastic constants for pentaerythritol tetranitrate single crystals](#)

[J. Appl. Phys.](#) **90**, 1669 (2001); 10.1063/1.1385352

[Erratum: "Effective secondorder elastic constants of a strained cubic crystal in the finite strain theory" \[J. Appl. Phys. 6 4, 3320 \(1988\)\]](#)

[J. Appl. Phys.](#) **65**, 405 (1989); 10.1063/1.343443

[Effective secondorder elastic constants of a strained cubic crystal in the finite strain theory](#)

[J. Appl. Phys.](#) **64**, 3320 (1988); 10.1063/1.341511

[The effective secondorder elastic constants of a strained crystal using the elastic wave propagation in a homogeneously deformed material](#)

[J. Appl. Phys.](#) **63**, 5728 (1988); 10.1063/1.340310



Effective second-order elastic constants of a strained crystal using the finite strain elasticity theory

R. Ramji Rao and A. Padmaja

Department of Physics, Indian Institute of Technology, Madras 600 036, India

(Received 30 January 1987; accepted for publication 2 March 1987)

The finite strain elasticity theory of Murnaghan has been used to derive the expressions for the effective second-order elastic constants of tetragonal, trigonal, orthorhombic, monoclinic, and triclinic crystals in their strained state in terms of the second- and third-order elastic constants of the respective crystals in their natural state. These expressions are employed to obtain the pressure derivatives of the effective second-order elastic constants of some trigonal and tetragonal crystals for which experimental second- and third-order elastic constant data are available.

I. INTRODUCTION

The experimental determination of the third-order elastic constants (TOEC) and the pressure derivatives of the effective second-order elastic constants (SOEC) of solids has received considerable attention in the last four decades as these are a measure of the anharmonicity of the solid. Elastic constants provide insight into the nature of the binding forces between the atoms since they are represented by the derivatives of the internal energy (adiabatic constants) or of the free energy (isothermal constants) of the crystal. The TOEC play an important role in solid-state physics because they determine the anharmonic properties of solids such as thermal expansion, temperature and pressure dependence of elastic constants, interaction of acoustic and thermal phonons, etc. The TOEC are also indispensable for the finite strain elasticity theory of Murnaghan¹ where the elastic stress is nonlinear with the elastic strain. However, in the literature, we find that theoretical calculations for the effective second-order elastic constants of a strained crystal had been performed only for the cubic² and the hexagonal³ crystals. Tables of $[2\partial(\rho_0\omega^2)/2\partial p]_{p=0}$ for various crystal classes except the triclinic and monoclinic systems have been presented by Brugger⁴ to obtain the TOEC of the solid.

The object of the present paper is to obtain expressions for the effective second-order elastic constants of tetragonal, trigonal, orthorhombic, monoclinic, and triclinic systems based on the finite strain elasticity theory in terms of the natural state SOEC and TOEC of the respective crystal systems. These expressions have been utilized to obtain the pressure derivatives of the effective SOEC of some trigonal and tetragonal crystals for which the experimental SOEC and TOEC are available. The basic importance of these expressions is that they enable one to fix up the first-order anharmonic parameters in the potential-energy expansion of a crystal in a lattice-dynamical model.

II. EFFECTIVE ELASTIC CONSTANTS OF A STRAINED CRYSTAL

Let us consider a triclinic crystal subjected to a hydrostatic pressure p . Let a_i be the coordinates of a material point in the natural state and X_i the coordinates of the same material point after applying the pressure. The Jacobian

$J = |\partial X_i / \partial a_j|$ is given by

$$J = \begin{vmatrix} (1 - \alpha_1) & 0 & 0 \\ 0 & (1 - \alpha_2) & 0 \\ 0 & 0 & (1 - \alpha_3) \end{vmatrix}, \quad (1)$$

where every line element along a_i is reduced in length by a factor $(1 - \alpha_i)$. In terms of the Lagrangian strain components η , ϵ , and ζ :

$$\begin{aligned} (1 - \alpha_1)^2 &= 1 + 2\eta, & (1 - \alpha_2)^2 &= 1 + 2\epsilon, \\ (1 - \alpha_3)^2 &= 1 + 2\zeta. \end{aligned} \quad (2)$$

The density ρ_0 in the natural state changes to ρ in the deformed state as

$$\rho/\rho_0 = 1/\det|J|. \quad (3)$$

An infinitesimal stress is superimposed on this deformed state. The final coordinates of the material particle are given by

$$x_i = X_i + \sum_j \beta_{ij} X_j, \quad (4)$$

where β_{ij} are the infinitesimal strain parameters. The Lagrangian strain parameters η_{ij} in the final state are given by

$$\eta_{ij} = \frac{1}{2} \sum_p \left(\frac{\partial x_p}{\partial a_i} \frac{\partial x_p}{\partial a_j} - \delta_{ij} \right) \quad (5)$$

and are obtained in terms of η , ϵ , ζ , and β_{ij} . The strain-energy density U can be written in powers of η_{ij} as

$$\begin{aligned} U &= \frac{1}{2} \sum_{ijkl} C_{ijkl} \eta_{ij} \eta_{kl} \\ &+ \frac{1}{6} \sum_{ijklmn} C_{ijklmn} \eta_{ij} \eta_{kl} \eta_{mn} + \dots \end{aligned} \quad (6)$$

The stress tensor in the final state is given by Murnaghan¹ as

$$\tau_{ij} = \frac{\rho}{\rho_0} \sum_{pq} \frac{\partial x_i}{\partial a_p} \frac{\partial U}{\partial \eta_{pq}} \frac{\partial x_j}{\partial a_q}. \quad (7)$$

The effective SOEC C_{ijpq}^1 can be obtained to the first order in the strains η , ϵ , and ζ by comparing Eq. (7) with

$$\tau_{ij} = -p\delta_{ij} + \sum_{kl} C_{ij,kl}^1 \beta_{kl}, \quad (8)$$

where p denotes the pressure. Thus we find for a triclinic crystal the following expressions for C_{ijkl}^1 .

A. Triclinic system

The triclinic crystal has 21 independent SOEC and 56 independent TOEC. The expressions for the 21 effective SOEC of the strained triclinic crystal are as follows:

$$C_{11}^1 = C_{11} + \eta(5C_{11} + C_{111}) + \epsilon(-C_{11} + 2C_{12} + C_{112}) + \zeta(-C_{11} + 2C_{13} + C_{113}), \quad (9)$$

$$C_{12}^1 = C_{12} + \eta(C_{12} + C_{112}) + \epsilon(C_{12} + C_{122}) + \zeta(-C_{12} + C_{123}), \quad (10)$$

$$C_{13}^1 = C_{13} + \eta(C_{13} + C_{113}) + \epsilon(-C_{13} + C_{123}) + \zeta(C_{13} + C_{133}), \quad (11)$$

$$C_{14}^1 = C_{14} + \eta(C_{14} + C_{114}) + C_{124}\epsilon + C_{134}\zeta, \quad (12)$$

$$C_{15}^1 = C_{15} + \eta(3C_{15} + C_{115}) + \epsilon(-C_{15} + C_{25} + C_{125}) + \zeta(C_{35} + C_{135}), \quad (13)$$

$$C_{16}^1 = C_{16} + \eta(3C_{16} + C_{116}) + \epsilon(C_{26} + C_{126}) + \zeta(-C_{16} + C_{36} + C_{136}), \quad (14)$$

$$C_{22}^1 = C_{22} + \eta(2C_{12} - C_{22} + C_{122}) + \zeta(5C_{22} + C_{222}) + \zeta(2C_{23} - C_{22} + C_{223}), \quad (15)$$

$$C_{23}^1 = C_{23} + \eta(-C_{23} + C_{123}) + \epsilon(C_{23} + C_{223}) + \zeta(C_{23} + C_{233}), \quad (16)$$

$$C_{24}^1 = C_{24} + \eta(C_{14} - C_{24} + C_{124}) + \epsilon(3C_{24} + C_{224}) + \zeta(C_{34} + C_{334}), \quad (17)$$

$$C_{25}^1 = C_{25} + C_{125}\eta + \epsilon(C_{25} + C_{225}) + C_{235}\zeta, \quad (18)$$

$$C_{26}^1 = C_{26} + \eta(C_{16} + 2C_{166} + C_{126}) + \epsilon(3C_{26} + 2C_{266} + C_{226}) + \zeta(C_{36} - C_{26} + C_{236} + 2C_{366}), \quad (19)$$

$$C_{33}^1 = C_{33} + \eta(2C_{13} - C_{33} + C_{133}) + \epsilon(2C_{23} - C_{33} + C_{233}) + \zeta(5C_{33} + C_{333}), \quad (20)$$

$$C_{34}^1 = C_{34} + \eta(C_{14} - C_{34} + C_{134}) + \epsilon(C_{24} + C_{234}) + \zeta(3C_{34} + C_{334}), \quad (21)$$

$$C_{35}^1 = C_{35} + \eta(C_{15} + C_{135}) + \epsilon(C_{25} - C_{35} + C_{235}) + \zeta(3C_{35} + C_{335}), \quad (22)$$

$$C_{36}^1 = C_{36} + C_{136}\eta + C_{236}\epsilon + (C_{36} + C_{336})\zeta, \quad (23)$$

$$C_{44}^1 = C_{44} + \eta(\frac{1}{2}C_{12} + \frac{1}{2}C_{13} - C_{44} + C_{144}) + \epsilon(\frac{1}{2}C_{22} + \frac{1}{2}C_{23} + C_{44} + C_{244}) + \zeta(\frac{1}{2}C_{23} + \frac{1}{2}C_{33} + C_{44} + C_{344}), \quad (24)$$

$$C_{45}^1 = C_{45} + \eta(\frac{1}{2}C_{16} + C_{145}) + \epsilon(\frac{1}{2}C_{26} + C_{245}) + \zeta(\frac{1}{2}C_{36} + C_{45} + C_{345}), \quad (25)$$

$$C_{46}^1 = C_{46} + \eta(\frac{1}{2}C_{15} + C_{146}) + \epsilon(\frac{1}{2}C_{25} + C_{46} + C_{246}) + \zeta(\frac{1}{2}C_{35} + C_{346}), \quad (26)$$

$$C_{55}^1 = C_{55} + \eta(\frac{1}{2}C_{11} + \frac{1}{2}C_{13} + C_{55} + C_{155}) + \epsilon(\frac{1}{2}C_{12} + \frac{1}{2}C_{23} - C_{55} + C_{255}) + \zeta(\frac{1}{2}C_{13} + \frac{1}{2}C_{33} + C_{55} + C_{355}), \quad (27)$$

$$C_{56}^1 = C_{56} + \eta(\frac{1}{2}C_{14} + C_{56} + C_{156}) + \epsilon(\frac{1}{2}C_{24} + C_{256}) + \zeta(\frac{1}{2}C_{34} + C_{356}), \quad (28)$$

$$C_{66}^1 = C_{66} + \eta(\frac{1}{2}C_{11} + \frac{1}{2}C_{12} + C_{66} + C_{166}) + \epsilon(\frac{1}{2}C_{12} + \frac{1}{2}C_{22} + C_{66} + C_{266}) + \zeta(\frac{1}{2}C_{13} + \frac{1}{2}C_{23} - C_{66} + C_{366}). \quad (29)$$

B. Monoclinic system

$$(2, m, 2/m)$$

The orthorhombic crystal has 9 independent SOEC and 20 independent TOEC. The expressions for the nine effective SOEC C_{11}^1 , C_{12}^1 , C_{13}^1 , C_{22}^1 , C_{23}^1 , C_{33}^1 , C_{44}^1 , C_{55}^1 , and C_{66}^1 are the same as the corresponding expressions for the triclinic crystal [see Eqs. (9), (10), (11), (15), (16), (20), (24), (27), and (29)]. η , ϵ , and ζ are given in terms of p and C_{ij} as

C. Orthorhombic system

$$\left(222, 2mm, \frac{2}{m} \frac{2}{m} \frac{2}{m}\right)$$

The monoclinic crystal has 13 independent SOEC and 32 independent TOEC. The expressions for the effective SOEC C_{11}^1 , C_{12}^1 , C_{13}^1 , C_{15}^1 , C_{22}^1 , C_{23}^1 , C_{25}^1 , C_{33}^1 , C_{35}^1 , C_{44}^1 , C_{46}^1 , C_{55}^1 , and C_{66}^1 are the same as the corresponding expressions for the triclinic crystal [see Eqs. (9)–(11), (13), (15), (16), (18), (20), (22), (24), (26), (27), and (29)].

$$|a| = \begin{vmatrix} C_{11} & C_{12} & C_{13} \\ C_{12} & C_{22} & C_{23} \\ C_{13} & C_{23} & C_{33} \end{vmatrix}, \quad \eta = -p \frac{\begin{vmatrix} 1 & C_{12} & C_{13} \\ 1 & C_{22} & C_{23} \\ 1 & C_{23} & C_{33} \end{vmatrix}}{|a|},$$

$$\epsilon = -p \frac{\begin{vmatrix} C_{11} & 1 & C_{13} \\ C_{12} & 1 & C_{23} \\ C_{13} & 1 & C_{33} \end{vmatrix}}{|a|} \quad \text{and} \quad \zeta = -p \frac{\begin{vmatrix} C_{11} & C_{12} & 1 \\ C_{12} & C_{22} & 1 \\ C_{13} & C_{23} & 1 \end{vmatrix}}{|a|}. \quad (30)$$

D. Tetragonal system

In the tetragonal system, the $4mm$, $\bar{4}2m$, 422 , $(4/m)$ ($2/m$) ($2/m$) classes have 6 independent SOEC and 12 independent TOEC and the 4 , $\bar{4}$ and $4/m$ classes have 7 independent SOEC and 16 independent TOEC. In the second group, the additional independent SOEC is C_{16} . The expressions for the seven effective SOEC are as follows:

$$C_{11}^1 = C_{11} + \eta(4C_{11} + 2C_{12} + C_{111} + C_{112}) + \zeta(-C_{11} + 2C_{13} + C_{113}), \quad (31)$$

$$C_{12}^1 = C_{12} + \eta(2C_{12} + 2C_{112}) + \zeta(-C_{12} + C_{123}), \quad (32)$$

$$C_{13}^1 = C_{13} + \eta(C_{113} + C_{123}) + \zeta(C_{13} + C_{133}), \quad (33)$$

$$C_{16}^1 = C_{16} + \eta(2C_{16} + C_{116}) + \zeta(-C_{16} + C_{136}), \quad (34)$$

$$C_{33}^1 = C_{33} + \eta(4C_{13} - 2C_{33} + 2C_{133}) + \zeta(5C_{33} + C_{333}), \quad (35)$$

$$C_{44}^1 = C_{44} + \eta(\frac{1}{2}C_{11} + \frac{1}{2}C_{12} + C_{13} + C_{144} + C_{155}) + \zeta(\frac{1}{2}C_{13} + \frac{1}{2}C_{33} + C_{44} + C_{344}), \quad (36)$$

$$C_{66}^1 = C_{66} + \eta(C_{11} + C_{12} + 2C_{66} + 2C_{166}) + \zeta(C_{13} - C_{66} + C_{366}). \quad (37)$$

E. Trigonal system

In the trigonal system, the $3m, 32, \bar{3} (2/m)$ classes have 6 independent SOEC and 14 independent TOEC and the $3, \bar{3}$ classes have 7 independent SOEC and 20 independent TOEC. The additional independent SOEC of the $3, \bar{3}$ classes is C_{15} .

The expressions for $C_{11}^1, C_{13}^1, C_{33}^1,$ and C_{44}^1 are the same as the corresponding expressions for the tetragonal system. [See Eqs. (31), (33), (35), and (36)]. The remaining equations are as follows:

$$C_{12}^1 = C_{12} + \eta(2C_{12} + C_{111} + 2C_{112} - C_{222}) + \zeta(-C_{12} + C_{123}), \quad (38)$$

$$C_{14}^1 = C_{14} + \eta(C_{14} + C_{114} + C_{124}) + C_{134}\zeta, \quad (39)$$

$$C_{66}^1 = C_{66} + \eta(2C_{11} - \frac{1}{2}C_{112} + \frac{1}{2}C_{222}) + \zeta(C_{13} - C_{66} + \frac{1}{2}C_{113} - \frac{1}{2}C_{123}) = \frac{1}{2}(C_{11}^1 - C_{12}^1), \quad (40)$$

$$C_{15}^1 = C_{15} + \eta(C_{15} + C_{115} + C_{125}) + C_{135}\zeta. \quad (41)$$

The Lagrangian strains η and ϵ are identical for the trigonal

and tetragonal crystals which are uniaxial:

$$\eta = \frac{(C_{13} - C_{33})p}{(C_{11} + C_{12})C_{33} - 2C_{13}^2},$$

$$\zeta = \frac{(2C_{13} - C_{11} - C_{12})p}{(C_{11} + C_{12})C_{33} - 2C_{13}^2}. \quad (42)$$

III. RESULTS AND DISCUSSION

The SOEC and the TOEC of Bismuth,⁵ α -quartz,⁶ calcite,⁷ alumina,^{8,9} lithium niobate,¹⁰ and tin¹¹ are available in the literature. The pressure derivatives of the effective SOEC of these six materials have been calculated using the present expressions. These along with the experimental values are presented in Table I. The agreement between the calculated and the experimental pressure derivatives is found to be satisfactory. The consistently low values of some of the calculated $\partial C_{ij}^1/\partial p$ can be attributed to the higher-order anharmonicity prevalent in these materials and to account for the differences one may have to include the fourth-order elastic constants (FOEC) in the expressions for C_{ij}^1 . The TOEC are related to the first-order anharmonic parameters while the FOEC are related to the second-order anharmonic parameters in the interatomic potential of the crystal. In tin,¹¹ it may be noted that there is a discrepancy in the value of $\partial C_{12}^1/\partial p$ obtained from the measured quantities

$$\frac{\partial}{\partial p} \left(\frac{1}{2}(C_{11}^1 + C_{12}^1) + C_{66}^1 \right)$$

and

$$\frac{\partial}{\partial p} \left(\frac{1}{2}(C_{11}^1 - C_{12}^1) \right)$$

by Swartz, Chua, and Elbaum.¹¹ The difference in the calculated and the experimental pressure derivatives of the effective

TABLE I. Values of $\partial C_{ij}^1/\partial p$. The first row against each crystal gives our present calculated values while the second row gives the experimental values with corresponding reference.

Serial no.	Crystal	$\frac{\partial C_{11}^1}{\partial p}$	$\frac{\partial C_{12}^1}{\partial p}$	$\frac{\partial C_{13}^1}{\partial p}$	$\frac{\partial C_{14}^1}{\partial p}$	$\frac{\partial C_{33}^1}{\partial p}$	$\frac{\partial C_{44}^1}{\partial p}$	$\frac{\partial C_{66}^1}{\partial p}$
1	Bismuth (Ref. 5)	5.31	1.85	4.38	1.96	5.73	3.36	1.73
		6.38	2.38	4.69	1.70	6.62	3.37	2.0
2	α -Quartz (Ref. 6)	2.26	7.58	4.92	1.89	9.74	2.63	-2.66
		3.28	8.66	5.97	1.93	10.84	2.66	-2.69
3	Calcite (Ref. 7)	2.00	1.04	2.19	-1.26	1.82	0.92	0.48
		3.02	2.05	3.19	-1.25	2.80	0.92	0.49
4	Alumina (Ref. 8)	5.16	2.22	2.61	0.11	3.99	2.21	1.47
		6.17	3.28	3.65	0.13	4.99	2.24	1.45
5	Lithium niobate	-4.45	-4.94	-4.93	+1.17	-1.04	+2.32	+0.24
	
6	Tin (Ref. 11)	6.48	5.61	2.96	...	8.87	2.22	1.61
		7.49	6.71	9.87	3.22	1.61

tive SOEC of tin could be attributed to the inconsistency in the value of $\partial C_{12}^1/\partial p$. In calcite, Kaga⁷ had measured the TOEC and the pressure derivatives at 0 °C while the SOEC presented are those at room temperature. The TOEC and the pressure derivatives of alumina had been measured by Geiske and Barsch^{8,9} and also by Hankey and Schuele¹² and both are in good agreement with each other. The values of Geiske and Barsch^{8,9} are used in the present calculations. The present expressions for C_{ij}^1 are useful to fix the first-order anharmonic parameters of the crystal potential in a lattice-dynamical model. These anharmonic parameters can be used to explain the anharmonic properties of the material. For example, one can calculate the generalized Gruneisen parameters (GPs) using these anharmonic parameters and thus obtain the thermal expansion of the material as a function of temperature.

ACKNOWLEDGMENT

One of us (A.P.) is grateful to the Indian Institute of Technology, Madras, for the award of a research fellowship.

- ¹F. D. Murnaghan, *Finite Deformation of an Elastic Solid* (Wiley, New York, 1951).
- ²F. Birch, *Phys. Rev.* **71**, 809 (1947).
- ³R. Ramji Rao and R. Srinivasan, *Phys. Status Solidi* **31**, K 39 (1969).
- ⁴K. Brugger, *J. Appl. Phys.* **36**, 768 (1965).
- ⁵T. Hailing and G. A. Saunders, *Philos. Mag.* **48**, 571 (1983).
- ⁶R. N. Thurston, H. J. McSkimin, and P. Andreatch, Jr., *J. Appl. Phys.* **37**, 267 (1966).
- ⁷H. Kaga, *Phys. Rev.* **172**, 900 (1968).
- ⁸J. H. Geiske and G. R. Barsch, *Phys. Status Solidi* **29**, 121 (1968).
- ⁹J. H. Geiske, *Diss. Abstr. (Penn State University)* **29**, 10 (1969).
- ¹⁰Y. Nakagawa, K. Yamanouchi, and K. Shibayama, *J. Appl. Phys.* **44**, 3969 (1973).
- ¹¹K. D. Swartz, W. B. Chua, and C. Elbaum, *Phys. Rev. B* **6**, 426 (1972).
- ¹²R. E. Hankey and D. E. Schuele, *J. Acoust. Soc. Am.* **48**, 190 (1970).