

The effective secondorder elastic constants of a strained crystal using the elastic wave propagation in a homogeneously deformed material

R. Ramji Rao and A. Padmaja

Citation: [Journal of Applied Physics](#) **63**, 5728 (1988); doi: 10.1063/1.340310

View online: <http://dx.doi.org/10.1063/1.340310>

View Table of Contents: <http://scitation.aip.org/content/aip/journal/jap/63/12?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.* **64**, 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

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

J. Appl. Phys. **62**, 440 (1987); 10.1063/1.339818



The effective second-order elastic constants of a strained crystal using the elastic wave propagation in a homogeneously deformed material

R. Ramji Rao^{a)}

Institute of Condensed Matter, University of Geneva, Geneva, Switzerland

A. Padmaja

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

(Received 19 May 1987; accepted for publication 26 January 1988)

The equation for elastic wave propagation in a homogeneously deformed crystal has been used to obtain the expressions for the effective second-order elastic constants of the seven crystal systems in terms of their natural second- and third-order elastic constants. These expressions are employed to obtain the pressure derivatives of the effective second-order elastic constants of some cubic crystals for which experimental data are available.

I. INTRODUCTION

Elastic constants provide insight into the nature of the binding forces between the atoms. The higher-order elastic constants, such as the third-order elastic constants (TOEC), are useful in the study of the anharmonic properties of solids such as the pressure variation of elastic constants. One needs a knowledge of the effective second-order elastic constants (SOEC) of the strained crystal to study its anharmonic properties. In this paper, the equation for elastic wave propagation in a homogeneously deformed crystal given by Thurston and Brugger¹ has been employed to derive expressions for the effective SOEC of the seven crystal systems. These formulas have been used to obtain the pressure derivatives of the effective SOEC of some cubic crystals for which experimental SOEC and TOEC are available.

A. Effective elastic constants of a strained crystal

The equation for elastic wave propagation in a homogeneously deformed crystal is given by Thurston and Brugger¹ as

$$\rho_0 W^2 u_i = \sum_{j,k,l} A_{ij,kl}^S s_k s_l u_j, \quad (1)$$

where ρ_0 is the density of the crystal in the unstrained state, W is the natural wave velocity in a direction having direction cosines s_k in the undeformed state, and u_j are the components of displacement from the strained state. To the first order in the strain $A_{ij,kl}^S$ is given by

$$A_{ij,kl}^S = C_{ik,jl} + \sum_{m,n} \epsilon_{mn} (C_{ik,jl,mn} + C_{ik,ni} \delta_{mj} + C_{nk,jl} \delta_{mi} + C_{kl,mn} \delta_{ij}). \quad (2)$$

The $C_{ik,jl}$ are the adiabatic SOEC in the undeformed state and $C_{ik,jl,mn}$ are the TOEC in the notation of Brugger,¹ determined by measuring the changes in wave velocity under isothermal strain. ϵ_{mn} are the Lagrangian strains. The strains employed are ϵ_{11} , ϵ_{22} , and ϵ_{33} , which leave the crystal symmetry unaltered and are consistent with the hydrostatic and uniaxial stresses used in the measurement of the pressure derivatives of SOEC of a crystal. The natural wave ve-

locities W in any direction are determined by solving the determinantal equation

$$|\rho_0 W^2 \delta_{ij} - D'_{ij}| = 0, \quad (3)$$

where the strained matrix element D'_{ij} is given by

$$D'_{ij} = \sum_{k,l} s_k s_l A_{ij,kl}^S. \quad (4)$$

If we set $\epsilon_{mn} = 0$, we obtain the unstrained matrix elements as

$$D_{ij} = \sum_{k,l} s_k s_l C_{ik,jl}. \quad (5)$$

The symmetry of the crystal is preserved when it is subjected to a homogeneous deformation. Following Eq. (5), we write the strained matrix element D'_{ij} as

$$D'_{ij} = \sum_{k,l} s_k s_l C_{ik,jl}^1, \quad (6)$$

where $C_{ik,jl}^1$ is the effective SOEC of the strained crystal and is the coefficient of $(s_k s_l)$. Comparing Eqs. (4) and (6), we obtain expressions for $C_{ij,kl}^1$ in terms of the natural SOEC and TOEC of the crystal, to the first order in strains ϵ_{11} , ϵ_{22} , and ϵ_{33} . It may be noted that the effective SOEC do not have the same symmetry as the conventional (natural) SOEC. This implies that $C_{ik,jl}^1 \neq C_{ki,jl}^1$. However, $C_{ik,jl}^1 = C_{jl,ik}^1$ (pairwise interchange).

1. Triclinic system (1, $\bar{1}$)

There are 21 independent SOEC and 56 independent TOEC for a triclinic crystal. The expressions for the 45 effective SOEC are given here. The condensed Voigt notation is used for the natural SOEC and TOEC in these expressions:

$$C_{11,11}^1 = C_{11} + \epsilon_{11}(C_{111} + 3C_{11}) + \epsilon_{22}(C_{112} + C_{12}) + \epsilon_{33}(C_{113} + C_{13}), \quad (7)$$

$$C_{11,22}^1 = C_{12} + \epsilon_{11}(C_{112} + C_{12}) + \epsilon_{22}(C_{122} + C_{12}) + \epsilon_{33}(C_{123}), \quad (8)$$

$$C_{11,33}^1 = C_{13} + \epsilon_{11}(C_{113} + C_{13}) + \epsilon_{22}(C_{123}) + \epsilon_{33}(C_{133} + C_{13}), \quad (9)$$

^{a)} On sabbatical leave from the Department of Physics, Indian Institute of Technology, Madras 600 036, India.

$$\begin{aligned}
C_{11,23}^1 &= C_{14} + \epsilon_{11}(C_{114} + C_{14}) \\
&\quad + \epsilon_{22}(C_{124} + C_{14}) + \epsilon_{33}(C_{134}), \quad (10) \\
C_{11,32}^1 &= C_{14} + \epsilon_{11}(C_{114} + C_{14}) \\
&\quad + \epsilon_{22}(C_{124}) + \epsilon_{33}(C_{134} + C_{14}), \quad (11) \\
C_{11,13}^1 &= C_{15} + \epsilon_{11}(C_{115} + 3C_{15}) \\
&\quad + \epsilon_{22}(C_{125} + C_{25}) + \epsilon_{33}(C_{135} + C_{35}), \quad (12) \\
C_{11,31}^1 &= C_{15} + \epsilon_{11}(C_{115} + C_{15}) + \epsilon_{22}(C_{125}) \\
&\quad + \epsilon_{33}(C_{135} + C_{15}), \quad (13) \\
C_{11,12}^1 &= C_{16} + \epsilon_{11}(C_{116} + 3C_{16}) \\
&\quad + \epsilon_{22}(C_{126} + C_{26}) + \epsilon_{33}(C_{136} + C_{36}), \quad (14) \\
C_{11,21}^1 &= C_{16} + \epsilon_{11}(C_{116} + C_{16}) \\
&\quad + \epsilon_{22}(C_{126} + C_{16}) + \epsilon_{33}(C_{136}), \quad (15) \\
C_{22,22}^1 &= C_{22} + \epsilon_{11}(C_{122} + C_{12}) + \epsilon_{22}(C_{222} + 3C_{22}) \\
&\quad + \epsilon_{33}(C_{223} + C_{23}), \quad (16) \\
C_{22,33}^1 &= C_{23} + \epsilon_{11}(C_{123}) + \epsilon_{22}(C_{223} + C_{23}) \\
&\quad + \epsilon_{33}(C_{233} + C_{23}), \quad (17) \\
C_{22,23}^1 &= C_{24} + \epsilon_{11}(C_{124} + C_{14}) + \epsilon_{22}(C_{224} + 3C_{24}) \\
&\quad + \epsilon_{33}(C_{234} + C_{34}), \quad (18) \\
C_{22,32}^1 &= C_{24} + \epsilon_{11}(C_{124}) + \epsilon_{22}(C_{224} + C_{24}) \\
&\quad + \epsilon_{33}(C_{234} + C_{24}), \quad (19) \\
C_{22,13}^1 &= C_{25} + \epsilon_{11}(C_{125} + C_{25}) \\
&\quad + \epsilon_{22}(C_{225} + C_{25}) + \epsilon_{33}(C_{235}), \quad (20) \\
C_{22,31}^1 &= C_{25} + \epsilon_{11}(C_{125}) + \epsilon_{22}(C_{225} + C_{25}) \\
&\quad + \epsilon_{33}(C_{235} + C_{25}), \quad (21) \\
C_{22,12}^1 &= C_{26} + \epsilon_{11}(C_{126} + C_{26}) \\
&\quad + \epsilon_{22}(C_{226} + C_{26}) + \epsilon_{33}(C_{236}), \quad (22) \\
C_{22,21}^1 &= C_{26} + \epsilon_{11}(C_{126} + C_{16}) + \epsilon_{22}(C_{226} + 3C_{26}) \\
&\quad + \epsilon_{33}(C_{236} + C_{36}), \quad (23) \\
C_{33,33}^1 &= C_{33} + \epsilon_{11}(C_{133} + C_{13}) + \epsilon_{22}(C_{233} + C_{23}) \\
&\quad + \epsilon_{33}(C_{333} + 3C_{33}), \quad (24) \\
C_{33,23}^1 &= C_{34} + \epsilon_{11}(C_{134}) + \epsilon_{22}(C_{234} + C_{34}) \\
&\quad + \epsilon_{33}(C_{334} + C_{34}), \quad (25) \\
C_{33,32}^1 &= C_{34} + \epsilon_{11}(C_{134} + C_{14}) + \epsilon_{22}(C_{234} + C_{24}) \\
&\quad + \epsilon_{33}(C_{334} + 3C_{34}), \quad (26) \\
C_{33,13}^1 &= C_{35} + \epsilon_{11}(C_{135} + C_{35}) \\
&\quad + \epsilon_{22}(C_{235}) + \epsilon_{33}(C_{335} + C_{35}), \quad (27) \\
C_{33,31}^1 &= C_{35} + \epsilon_{11}(C_{135} + C_{15}) + \epsilon_{22}(C_{235} + C_{25}) \\
&\quad + \epsilon_{33}(C_{335} + 3C_{35}), \quad (28) \\
C_{32,12}^1 &= C_{36} + \epsilon_{11}(C_{136} + C_{36}) + \epsilon_{22}(C_{236}) \\
&\quad + \epsilon_{33}(C_{336} + C_{36}), \quad (29) \\
C_{33,21}^1 &= C_{36} + \epsilon_{11}(C_{136}) + \epsilon_{22}(C_{236} + C_{36}) \\
&\quad + \epsilon_{33}(C_{336} + C_{36}), \quad (30) \\
C_{23,23}^1 &= C_{44} + \epsilon_{11}(C_{144} + C_{13}) + \epsilon_{22}(C_{244} \\
&\quad + 2C_{44} + C_{23}) + \epsilon_{33}(C_{344} + C_{33}), \quad (31) \\
C_{23,32}^1 &= C_{44} + \epsilon_{11}(C_{144}) + \epsilon_{22}(C_{244} + C_{44}) \\
&\quad + \epsilon_{33}(C_{344} + C_{44}), \quad (32) \\
C_{32,32}^1 &= C_{44} + \epsilon_{11}(C_{144} + C_{12}) + \epsilon_{22}(C_{244} + C_{22}) \\
&\quad + \epsilon_{33}(C_{344} + 2C_{44} + C_{23}), \quad (33) \\
C_{32,13}^1 &= C_{45} + \epsilon_{11}(C_{145} + C_{45}) + \epsilon_{22}(C_{245}) \\
&\quad + \epsilon_{33}(C_{345} + C_{45}), \quad (34) \\
C_{32,31}^1 &= C_{45} + \epsilon_{11}(C_{145} + C_{16}) + \epsilon_{22}(C_{245} + C_{26}) \\
&\quad + \epsilon_{33}(C_{345} + 2C_{45} + C_{36}), \quad (35) \\
C_{23,31}^1 &= C_{45} + \epsilon_{11}(C_{145}) + \epsilon_{22}(C_{245} + C_{45}) \\
&\quad + \epsilon_{33}(C_{345} + C_{45}), \quad (36) \\
C_{23,13}^1 &= C_{45} + \epsilon_{11}(C_{145} + C_{45}) + \epsilon_{22}(C_{245} + C_{45}) \\
&\quad + \epsilon_{33}(C_{345}), \quad (37) \\
C_{23,12}^1 &= C_{46} + \epsilon_{11}(C_{146} + C_{46}) \\
&\quad + \epsilon_{22}(C_{246} + C_{46}) + \epsilon_{33}(C_{346}), \quad (38) \\
C_{23,21}^1 &= C_{46} + \epsilon_{11}(C_{146} + C_{15}) + \epsilon_{22}(C_{246} + 2C_{46} \\
&\quad + C_{25}) + \epsilon_{33}(C_{346} + C_{35}), \quad (39) \\
C_{32,21}^1 &= C_{46} + \epsilon_{11}(C_{146}) + \epsilon_{22}(C_{246} + C_{46}) \\
&\quad + \epsilon_{33}(C_{346} + C_{46}), \quad (40) \\
C_{32,12}^1 &= C_{46} + \epsilon_{11}(C_{146} + C_{46}) + \epsilon_{22}(C_{246}) \\
&\quad + \epsilon_{33}(C_{346} + C_{46}), \quad (41) \\
C_{13,13}^1 &= C_{55} + \epsilon_{11}(C_{155} + 2C_{55} + C_{13}) \\
&\quad + \epsilon_{22}(C_{255} + C_{23}) + \epsilon_{33}(C_{355} + C_{33}), \quad (42) \\
C_{13,31}^1 &= C_{55} + \epsilon_{11}(C_{155} + C_{55}) + \epsilon_{22}(C_{255}) \\
&\quad + \epsilon_{33}(C_{355} + C_{55}), \quad (43) \\
C_{31,31}^1 &= C_{55} + \epsilon_{11}(C_{155} + C_{11}) + \epsilon_{22}(C_{255} + C_{12}) \\
&\quad + \epsilon_{33}(C_{355} + 2C_{55} + C_{13}), \quad (44) \\
C_{13,12}^1 &= C_{56} + \epsilon_{11}(C_{156} + 2C_{56} + C_{14}) \\
&\quad + \epsilon_{22}(C_{256} + C_{24}) + \epsilon_{33}(C_{356} + C_{34}), \quad (45) \\
C_{13,21}^1 &= C_{56} + \epsilon_{11}(C_{156} + C_{56}) \\
&\quad + \epsilon_{22}(C_{256} + C_{56}) + \epsilon_{33}(C_{356}), \quad (46) \\
C_{31,12}^1 &= C_{56} + \epsilon_{11}(C_{156} + C_{56}) + \epsilon_{22}(C_{256}) \\
&\quad + \epsilon_{33}(C_{356} + C_{56}), \quad (47) \\
C_{31,21}^1 &= C_{56} + \epsilon_{11}(C_{156}) + \epsilon_{22}(C_{256} + C_{56}) \\
&\quad + \epsilon_{33}(C_{356} + C_{56}), \quad (48) \\
C_{12,12}^1 &= C_{66} + \epsilon_{11}(C_{166} + 2C_{66} + C_{12}) \\
&\quad + \epsilon_{22}(C_{266} + C_{22}) + \epsilon_{33}(C_{366} + C_{23}), \quad (49) \\
C_{12,21}^1 &= C_{66} + \epsilon_{11}(C_{166} + C_{66}) \\
&\quad + \epsilon_{22}(C_{266} + C_{66}) + \epsilon_{33}(C_{366}), \quad (50) \\
C_{21,21}^1 &= C_{66} + \epsilon_{11}(C_{166} + C_{11}) + \epsilon_{22}(C_{266} + 2C_{66} \\
&\quad + C_{12}) + \epsilon_{33}(C_{366} + C_{13}), \quad (51)
\end{aligned}$$

The Lagrangian strains ϵ_{11} , ϵ_{22} , and ϵ_{33} can be expressed in terms of the pressure p and the elastic constants C_{ij} :

$$|a| = \begin{vmatrix} C_{11} & C_{12} & C_{13} \\ C_{12} & C_{22} & C_{23} \\ C_{13} & C_{23} & C_{33} \end{vmatrix},$$

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

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

$$\epsilon_{33} = -p \frac{\begin{vmatrix} C_{11} & C_{12} & 1 \\ C_{12} & C_{22} & 1 \\ C_{13} & C_{23} & 1 \end{vmatrix}}{|a|}. \quad (52)$$

2. Monoclinic system (2,m,2/m)

The monoclinic crystal has 13 independent SOEC and 32 independent TOEC. The expressions for the 25 effective SOEC, viz.,

$$C_{11,11}^1, C_{11,22}^1, C_{11,33}^1, C_{11,13}^1, C_{11,31}^1, C_{22,22}^1, \\ C_{22,33}^1, C_{22,13}^1, C_{22,31}^1, C_{33,33}^1, C_{33,13}^1, C_{33,31}^1, \\ C_{23,23}^1, C_{23,32}^1, C_{32,32}^1, C_{23,12}^1, C_{23,21}^1, C_{32,12}^1, \\ C_{32,21}^1, C_{13,13}^1, C_{13,31}^1, C_{31,31}^1, C_{12,12}^1, C_{12,21}^1, C_{21,21}^1$$

are the same as the corresponding expressions for the triclinic crystal.

3. Orthorhombic system (222,mm2,2/m 2/m 2/m)

The orthorhombic crystal has nine independent SOEC and 20 independent TOEC. The expressions for the 15 effective SOEC, viz.,

$$C_{11,11}^1, C_{11,22}^1, C_{11,33}^1, C_{22,22}^1, C_{22,33}^1, C_{33,33}^1, C_{23,23}^1, \\ C_{23,32}^1, C_{32,32}^1, C_{13,13}^1, C_{13,31}^1, C_{31,31}^1, C_{12,12}^1, C_{12,21}^1, C_{21,21}^1$$

are the same as the corresponding expressions for the triclinic crystal.

4. Tetragonal system (4mm, $\bar{4}2m$, 422, 4/m 2/m 2/m, $4\bar{4}4/m$)

In the tetragonal system, the 4mm, $\bar{4}2m$, 422, and 4/m 2/m 2/m, classes have six independent SOEC and 12 independent TOEC while the $4\bar{4}4/m$ group has seven independent SOEC and 16 independent TOEC. In the second group the additional independent SOEC is C_{16} . The expressions for the ten effective SOEC are given below. The Lagrangian strains ϵ_{11} and ϵ_{22} are equal for uniaxial crystals—tetragonal, trigonal, and hexagonal.

$$C_{11,11}^1 = C_{11} + \epsilon_{11}(C_{111} + C_{112} + 3C_{11} + C_{12}) \\ + \epsilon_{33}(C_{113} + C_{13}), \quad (53)$$

$$C_{11,22}^1 = C_{12} + \epsilon_{11}(2C_{112} + 2C_{12}) + \epsilon_{33}(C_{123}), \quad (54)$$

$$C_{11,33}^1 = C_{13} + \epsilon_{11}(C_{113} + C_{123} + C_{13}) \\ + \epsilon_{33}(C_{133} + C_{13}), \quad (55)$$

$$C_{11,12}^1 = C_{16} + \epsilon_{11}(C_{116} + 2C_{16}) + \epsilon_{33}(C_{136}), \quad (56)$$

$$C_{33,33}^1 = C_{33} + \epsilon_{11}(2C_{133} + 2C_{13}) \\ + \epsilon_{33}(C_{333} + 3C_{33}), \quad (57)$$

$$C_{23,23}^1 = C_{44} + \epsilon_{11}(C_{144} + C_{155} + 2C_{13} + 2C_{44}) \\ + \epsilon_{33}(C_{344} + C_{33}), \quad (58)$$

$$C_{32,32}^1 = C_{44} + \epsilon_{11}(C_{144} + C_{155} + C_{11} + C_{12}) \\ + \epsilon_{33}(C_{344} + 2C_{44} + C_{13}), \quad (59)$$

$$C_{23,32}^1 = C_{44} + \epsilon_{11}(C_{144} + C_{155} + C_{44}) \\ + \epsilon_{33}(C_{344} + C_{44}), \quad (60)$$

$$C_{12,12}^1 = C_{66} + \epsilon_{11}(2C_{166} + 2C_{66} + C_{11} + C_{12}) \\ + \epsilon_{33}(C_{366} + C_{13}), \quad (61)$$

$$C_{12,21}^1 = C_{66} + \epsilon_{11}(2C_{166} + 2C_{66}) + \epsilon_{33}(C_{366}). \quad (62)$$

The following interrelations hold for the tetragonal system:

$$C_{22,22}^1 = C_{11,11}^1, \quad C_{22,33}^1 = C_{11,33}^1, \\ C_{22,12}^1 = -C_{11,12}^1, \quad C_{13,13}^1 = C_{23,23}^1, \\ C_{31,31}^1 = C_{32,32}^1, \quad C_{31,13}^1 = C_{32,23}^1. \quad (63)$$

5. Hexagonal system (622, 6mm, $\bar{6}m2$, 6/m 2/m 2/m, $6\bar{6}6/m$)

In the hexagonal system, the classes 622, 6mm, $\bar{6}m2$, 6/m 2/m 2/m have five independent SOEC and ten independent TOEC. The group $6\bar{6}6/m$ has five independent SOEC and 12 independent TOEC. The effective SOEC $C_{11,11}^1$, $C_{11,33}^1$, $C_{23,23}^1$, $C_{23,32}^1$, $C_{32,32}^1$, and $C_{33,33}^1$ are given by the corresponding expressions of the tetragonal system.

The remaining effective SOEC are

$$C_{11,22}^1 = C_{12} + \epsilon_{11}(C_{111} + 2C_{112} - C_{222} + 2C_{12}) \\ + \epsilon_{33}(C_{123}), \quad (64)$$

$$C_{12,12}^1 = C_{66} + \epsilon_{11}\{[(C_{222} - C_{112})/2] + 2C_{11}\} \\ + \epsilon_{33}\{[(C_{113} - C_{123})/2] + C_{13}\}, \quad (65)$$

$$C_{12,21}^1 = C_{66} + \epsilon_{11}\{[(C_{222} - C_{112})/2] + 2C_{66}\} \\ + \epsilon_{33}\{[(C_{113} - C_{123})/2]\}. \quad (66)$$

The interrelations for the tetragonal system hold for hexagonal systems also.

6. Trigonal system (32, 3m, $\bar{3}2/m$, $3\bar{3}$)

The classes 32, 3m, and $\bar{3}2/m$ have six independent SOEC and 14 independent TOEC and the $3\bar{3}$ class has seven independent SOEC and 20 independent TOEC. The additional independent SOEC of the $3\bar{3}$ group is C_{15} . The expressions for the effective SOEC, $C_{11,11}^1$, $C_{11,22}^1$, $C_{11,33}^1$, $C_{33,33}^1$, $C_{23,23}^1$, $C_{32,32}^1$, $C_{23,32}^1$, $C_{12,12}^1$, and $C_{12,21}^1$ are the same as

those for the hcp system. The remaining effective SOEC are

$$C_{11,23}^I = C_{14} + \epsilon_{11}(C_{114} + C_{124} + 2C_{14}) + \epsilon_{33}(C_{134}), \quad (67)$$

$$C_{11,32}^I = C_{14} + \epsilon_{11}(C_{114} + C_{124} + C_{14}) + \epsilon_{33}(C_{134} + C_{14}), \quad (68)$$

$$C_{11,13}^I = C_{15} + \epsilon_{11}(C_{115} + C_{125} + 2C_{15}) + \epsilon_{33}(C_{135}), \quad (69)$$

$$C_{11,31}^I = C_{15} + \epsilon_{11}(C_{115} + C_{125} + C_{15}) + \epsilon_{33}(C_{135} + C_{15}). \quad (70)$$

The following interrelations hold true for the trigonal system:

$$\begin{aligned} C_{22,22}^I &= C_{11,11}^I, & C_{22,33}^I &= C_{11,33}^I, \\ C_{22,23}^I &= -C_{11,23}^I, & C_{22,32}^I &= C_{11,32}^I, \\ C_{22,13}^I &= -C_{11,13}^I, & C_{22,31}^I &= -C_{11,31}^I, \\ C_{23,12}^I &= C_{23,21}^I = -C_{11,13}^I, & C_{32,12}^I &= C_{32,21}^I, \\ C_{32,21}^I &= -C_{11,31}^I, & C_{13,13}^I &= C_{23,23}^I, \\ C_{13,31}^I &= C_{23,32}^I, & C_{31,31}^I &= C_{32,32}^I, \\ C_{13,12}^I &= C_{13,21}^I = C_{11,23}^I, & C_{31,12}^I &= C_{31,21}^I = C_{11,32}^I. \end{aligned} \quad (71)$$

The Lagrangian strains ϵ_{11} and ϵ_{33} for the uniaxial crystals are given by

$$\begin{aligned} \epsilon_{11} &= [(C_{13} - C_{33})P] / [(C_{11} + C_{12})C_{33} - 2C_{13}^2], \\ \epsilon_{33} &= [(2C_{13} - C_{11} - C_{12})P] / [(C_{11} + C_{12})C_{33} - 2C_{13}^2]. \end{aligned} \quad (72)$$

7. Cubic system ($\bar{4}32$, $\bar{4}3m$, $4/m\bar{3}2/m$, 23 , $2/m\bar{3}$)

The classes $\bar{4}32$, $\bar{4}3m$, and $4/m\bar{3}2/m$ (CI) have three independent SOEC and six independent TOEC, and the classes 23 and $2/m\bar{3}$ (CII) have three independent SOEC and eight independent TOEC. The expressions for the four effective SOEC are given below:

$$\begin{aligned} C_{11,11}^I &= C_{11} + \frac{\epsilon}{3}(C_{111} + 2C_{112} + 3C_{11} + 2C_{12}) \quad \text{for CI} \\ &= C_{11} + \frac{\epsilon}{3}(C_{111} + C_{112} + C_{113} + 3C_{11} + 2C_{12}) \\ &\quad \text{for CII,} \end{aligned} \quad (73)$$

$$\begin{aligned} C_{11,22}^I &= C_{12} + \frac{\epsilon}{3}(2C_{112} + C_{123} + 2C_{12}) \quad \text{for CI} \\ &= C_{12} + \frac{\epsilon}{3}(C_{112} + C_{113} + C_{123} + 2C_{12}) \quad \text{for CII,} \end{aligned} \quad (74)$$

$$\begin{aligned} C_{12,12}^I &= C_{44} + \frac{\epsilon}{3}(C_{144} + 2C_{155} + 2C_{44} + 2C_{12} + C_{11}) \\ &\quad \text{for CI,} \\ &= C_{44} + \frac{\epsilon}{3}(C_{144} + C_{155} + C_{166} + 2C_{44} \\ &\quad + 2C_{12} + C_{11}) \quad \text{for CII,} \end{aligned} \quad (75)$$

$$\begin{aligned} C_{12,21}^I &= C_{44} + \frac{\epsilon}{3}(C_{144} + 2C_{155} + 2C_{44}) \quad \text{for CI} \\ &= C_{44} + \frac{\epsilon}{3}(C_{144} + C_{155} + C_{166} + 2C_{44}) \quad \text{for CII.} \end{aligned} \quad (76)$$

ϵ is the uniform volume strain given by

$$\epsilon = -3P / (C_{11} + 2C_{12}) \quad (77)$$

under a hydrostatic pressure P . The following interrelations hold for the cubic system:

$$\begin{aligned} C_{11,11}^I &= C_{22,22}^I = C_{33,33}^I, \\ C_{12,12}^I &= C_{23,23}^I = C_{13,13}^I, \\ C_{12,21}^I &= C_{23,32}^I = C_{13,31}^I, \\ C_{11,22}^I &= C_{11,33}^I = C_{22,33}^I. \end{aligned} \quad (78)$$

II. RESULTS AND DISCUSSION

The derived formulas for cubic crystals have been employed to obtain the pressure derivatives of the effective second-order elastic constants of 17 cubic crystals. These are presented in Table I along with the corresponding experimental data.

TABLE I. Values of the pressure derivatives for some cubic crystals. The first line gives the present calculated values and the second line gives the experimental values. Reference for the SOEC, TOEC, and $\partial C_{ij,kl}^I / \partial P$ are also given in the second line.

Serial No.	Crystal	$\frac{\partial C_{11,11}^I}{\partial P}$	$\frac{\partial C_{11,22}^I}{\partial P}$	$\frac{\partial C_{23,23}^I}{\partial P}$
1	Cu	5.32	3.54	2.47
	Ref. 2	5.73	4.98	2.63
2	Ag	4.45	2.26	2.71
	Ref. 2	4.85	3.35	3.04
3	Au	5.12	3.36	1.36
	Ref. 2	5.72	4.96	1.52
4	Al	5.55	2.08	1.84
	Ref. 3	6.35	3.45	2.10
5	Li	3.01	1.96	0.67
	Ref. 4,5	3.36	3.26	0.93
6	Na	3.71	2.31	1.47
	Ref. 4,6	4.12	3.64	1.69
7	K	3.92	2.48	1.43
	Ref. 4,7	4.31	3.80	1.62
8	Rb	3.59	2.19	1.26
	Ref. 4,8	3.96	3.50	1.48
9	GaSb	4.41	3.43	0.75
	Ref. 9	4.93	4.66	1.00
10	GaAs	4.12	3.20	0.84
	Ref. 10	4.63	4.42	1.10
11	InSb	3.28	2.82	0.19
	Ref. 11			
12	NaCl	10.29	0.38	-0.13
	Ref. 12	11.62	1.58	+0.10
13	KCl	11.59	0.42	-0.70
	Ref. 12	13.00	1.56	-0.56
14	LiF	7.24	1.32	0.59
	Ref. 12	8.18	2.60	1.00
15	NaF	11.58	1.46	+0.13
	Ref. 13	12.70	2.50	+0.28
16	CaF ₂	5.82	3.84	0.92
	Ref. 14	6.05	4.35	1.31
17	BaF ₂	5.02	4.36	0.49
	Refs. 14 and 15	4.82	5.17	0.78

The noble metals Cu, Ag, Au, and Al may be grouped together in that the agreement between calculation and measurement is fair to 12%, except for $\partial C_{11,22}^1/\partial P$. The $\partial C_{11,22}^1/\partial P$ is consistently lower than the experimental value for all 17 crystals attempted here. The experimental TOEC are not available for the alkali metals and the theoretical TOEC values of Ramji Rao and Rajput⁴ have been used to obtain their pressure derivatives. The agreement with the experimental values for $\partial C_{11,11}^1/\partial P$ and $\partial C_{23,23}^1/\partial P$ is good to within 15%. In the semiconducting compounds GaSb and GaAs, the calculated values agree with those of experiment to within 28%. The alkali halides NaCl, KCl, LiF, and NaF and the alkaline-earth fluorides CaF₂ and BaF₂ fall into one group in the sense that in these crystals, the pressure derivative $\partial C_{23,23}^1/\partial P$ is in poor agreement with the experimental value.

The above disparities may be attributed to the second-order anharmonicity prevalent in these crystals and the inclusion of the fourth-order elastic constants (FOEC) may help to bring the calculated values closer to the experimental values. Incidentally the present work brings out the need to measure the FOEC of crystals at the earliest if one wants to explain the anharmonic properties of solids with accuracy.

The present formulas for $C_{ij,kl}^1$ can be used to evaluate the first-order anharmonic parameters of the crystal potential in a lattice-dynamical model, as the TOEC are a measure of the first-order anharmonicity in the crystal. These first-

order anharmonic parameters can be used to explain the anharmonic properties of the solid such as thermal expansion.

ACKNOWLEDGMENTS

The authors thank Professor M. Peter and Dr. E. Walker for their interest in this work. One of us (A.P.) is grateful to the Indian Institute of Technology, Madras, for the award of a research fellowship.

¹R. N. Thurston and K. Brugger, Phys. Rev. **133**, A1604 (1964); K. Brugger, *ibid.* **133**, A1611 (1964).

²Y. Hiki and A. V. Granato, Phys. Rev. **144**, 411 (1966).

³J. F. Thomas, Jr., Phys. Rev. **175**, 955 (1968).

⁴R. Ramji Rao and A. Rajput, Phys. Status Solidi B **94**, 691 (1979).

⁵J. P. Day and A. L. Ruoff, Phys. Status Solidi A **25**, 205 (1974).

⁶R. H. Martinson, Phys. Rev. **178**, 902 (1969).

⁷P. A. Smith and C. S. Smith, J. Phys. Chem. Solids **26**, 279 (1965).

⁸A. Pauer Lyle, Office of U.S. Naval Research Tech. Report No. 11 [quoted in R. Srinivasan and K. S. Girirajan, J. Phys. Chem. Solids **34**, 611 (1973)].

⁹V. Sundara Raja and P. J. Reddy, Phys. Lett. A **56**, 215 (1976).

¹⁰H. J. McSkimin and P. Andreatch, Jr., J. Appl. Phys. **38**, 2610 (1967).

¹¹J. R. Drabble and A. J. Brammer, Proc. Phys. Soc. London **91**, 959 (1967).

¹²J. R. Drabble and R. E. B. Strathen, Proc. Phys. Soc. London **92**, 1090 (1967).

¹³W. A. Bensch, Phys. Rev. B **6**, 1504 (1972).

¹⁴C. Wong and D. E. Schuele, J. Phys. Chem. Solids **28**, 1225 (1967).

¹⁵D. Gerlich, Phys. Rev. **168**, 947 (1968).