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Effective second-order elastic constants of a strained cubic crystal in the finite strain theory

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Expressions for the effective second-order elastic constants of a strained cubic crystal have been obtained using the finite strain theory of Murnaghan, in terms of the higher-order elastic constants of its natural state. These formulae are found to be different from those obtained by the earlier workers. These expressions are used to obtain the pressure derivatives of the effective second-order elastic constants of some cubic crystals for which experimental second- and third-order elastic constants are available. The second-order anharmonic contribution to the pressure derivatives of C^1_{11} and C^1_{12} of copper, silver, and gold is calculated from a knowledge of the estimated values of the fourth-order elastic constants of these metals.

The higher-order elastic constants of a crystal are useful in the study of its anharmonic properties and are related to the anharmonic coupling parameters of the crystal potential in a lattice dynamical model. The effective second-order elastic constants of a strained crystal constitute a useful tool in the study of its anharmonic properties such as the pressure and temperature variation of the second-order elastic constants. In this paper, expressions for the effective second-order elastic constants of a cubic crystal have been derived using the finite strain elasticity theory of Murnaghan[1] in terms of the natural state second-, third-, and fourth-order elastic constants (SOEC, TOEC, and FOEC).

Let us consider a cubic crystal subjected to a hydrostatic pressure "p." The coordinates a_i of a material particle in the natural state change to X_i after applying the pressure. The Jacobian of the transformation is

$$J = \mathrm{Det}\left(\frac{\partial X_i}{\partial a_j}\right) = \begin{vmatrix} (1-\alpha) & 0 & 0 \\ 0 & (1-\alpha) & 0 \\ 0 & 0 & (1-\alpha) \end{vmatrix}, \tag{1}$$

where every line element is reduced in length by a factor $(1-\alpha)$. In terms of the Lagrangian strain component η

$$(1-\alpha)^2 = 1 + 2\eta. \tag{2}$$

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

$$\rho/\rho_0 = 1/J. \tag{3}$$

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

$$x_i = X_i + \sum_j \beta_{ij} X_j, \tag{4}$$

where β_{ij} are the infinitesimal strain parameters. In the finite strain theory, the Lagrangian strain parameters in the final state are given by

$$\eta_{ij} = \frac{1}{2}\sum_{k=1}^{3}\left(\frac{\partial x_k}{\partial a_i}\frac{\partial x_k}{\partial a_j} - \delta_{ij}\right), \tag{5}$$

and are expressed in terms of η and β_{ij}. The symmetry relation $\eta_{ij} = \eta_{ji}$ is ignored here and only the first powers of β_{ij} are retained.

The strain energy density can be written in powers of η_{ij} as

$$U = \frac{1}{2}\sum_{ijkl} C_{ijkl}\eta_{ij}\eta_{kl} + \frac{1}{6}\sum_{ijklmn} C_{ijklmn}\eta_{ij}\eta_{kl}\eta_{mn} + \frac{1}{24}\sum_{ijklmnop} C_{ijklmnop}\eta_{ij}\eta_{kl}\eta_{mn}\eta_{op} + \cdots. \tag{6}$$

The stress tensor in the final state is given by

$$\tau_{ij} = \frac{\rho}{\rho_0}\sum_{kl}\frac{\partial x_i}{\partial a_k}\frac{\partial U}{\partial \eta_{kl}}\frac{\partial x_j}{\partial a_l}. \tag{7}$$

The effective SOEC C^1_{ijkl} of the crystal can be obtained to the second order in the strain η in terms of its natural SOEC, TOEC, and FOEC by comparing Eq. (7) with

$$\tau_{ij} = -p\delta_{ij} + \sum_{kl} C^1_{ijkl}\beta_{kl}. \tag{8}$$

Here δ_{ij} is the Kronecker delta. The (CI) Laue group of the cubic system has 3 SOEC, 6 TOEC, and 11 FOEC, respectively. The expressions for the effective SOEC of the cubic crystal are given below:

$$C^1_{11} = C_{11} + \eta(3C_{11} + 4C_{12} + C_{111} + 2C_{112}) + \eta^2(-\tfrac{5}{2}C_{11} - 4C_{12} + 2C_{111} + 8C_{112} + 2C_{123} + C_{1111} + 2C_{1112} + C_{1122} + C_{1123}), \tag{9}$$

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$$C_{12}^1 = C_{12} + \eta(C_{12} + 2C_{112} + C_{123}) + \eta^2(-\tfrac{1}{2}C_{12} + 2C_{112} + C_{123} + C_{1112} + C_{1122} + C_{1123}), \quad (10)$$

$$C_{44}^1 = C_{44} + \eta(C_{11} + 2C_{12} + C_{44} + C_{144} + 2C_{155}) + \eta^2(-C_{11} - 2C_{12} - \tfrac{1}{2}C_{44} + C_{111} + 3C_{112} + C_{123} + C_{144} + 2C_{155} + C_{1144} + C_{1155} + 2C_{4412} + C_{4423}). \quad (11)$$

A cubic crystal subjected to a hydrostatic pressure "p" will experience a uniform volume strain ϵ (negative) and η is given by

$$\eta = -(\epsilon/3) \text{ and } \epsilon = -3p/(C_{11} + 2C_{12}). \quad (12)$$

Birch[2] obtained expressions for the effective SOEC of a cubic crystal to the first degree in the Lagrangian strain and as such, these involve the natural second- and third-order elastic constants only. Ghate[3] derived expressions for the effective SOEC of a cubic crystal to the second degree in the Lagrangian strain involving its natural SOEC, TOEC, and FOEC. The present expressions for the effective SOEC of a cubic crystal have been obtained to the second degree in the Lagrangian strain including its natural SOEC, TOEC, and FOEC and these expressions differ from those of Birch[2] and of Ghate[3] in two respects:

(i) The numerical coefficients of the natural elastic constants involved in these expressions are, at times, different from those in the expressions derived by Birch[2] and Ghate.[3] This difference arises from an incorrect choice of the multiplicity factors associated with the elastic constants of various orders by these earlier authors.

(ii) There is omission or inclusion of some of the natural elastic constants in the expressions of Birch[2] and Ghate.[3]

Thurston and Brugger[4] derived expressions for the sound velocity in a homogeneously stressed material and for the stress derivatives of $(\rho_0 w^2)$ at zero stress, w being the natural velocity, in terms of its natural SOEC and TOEC. Brugger[5] presented thermodynamic definitions of the higher-order elastic coefficients of a thermoelastic medium in tensor and engineering notation. The notation of Brugger is used here in the definition of the higher-order elastic constants of a solid. Barron and Klein[6] derived expressions for the second-order elastic constants of a cubic solid under isotropic pressure in terms of the elastic energy density without explicit reference to higher-order elastic constants at any stage.

The present formulae have been employed to obtain the pressure derivatives of the effective SOEC of ten cubic crystals for which experimental TOEC are available. These are presented in Table I along with the available experimental pressure derivative data on these materials.

In all these ten crystals, the agreement of the pressure derivative of the C_{44}^1 with experiment is good as can be seen from Table I. This implies that the first-order anharmonicity (TOEC) is sufficient to corroborate the experimental pressure derivative of C_{44}^1 in all these ten materials and that there is no need of calculating the contribution arising from the second-order anharmonicity (FOEC). In the noble metals Cu, Ag, and Au,[7] the pressure derivatives of C_{11}^1 and C_{12}^1 deviate from the measured values by a maximum of 29% when only the first-order anharmonicity (TOEC) is taken into account. In Al,[8] the pressure derivative of C_{11}^1 differs from the measured value by 21% and that of C_{12}^1 differs by 32%. In GaSb,[9,10] the pressure derivatives of C_{11}^1 and C_{12}^1 deviate from the respective experimental values by 21%. The direct experimental pressure derivatives of GaAs (Ref. 11) and InSb (Ref. 12) are not available to make a comparison.

TABLE I. Values of the pressure derivatives of the effective SOEC for some cubic crystals. The first line gives the present calculated values and the second line gives the experimental values, if available. References for the SOEC, TOEC, and the pressure derivatives are also given in the second line.

Serial no.	Crystal	$\frac{\partial C_{11}^1}{\partial p}$	$\frac{\partial C_{12}^1}{\partial p}$	$\frac{\partial C_{44}^1}{\partial p}$
1	Cu	4.73	3.83	2.66
	Ref. 7	5.94	5.19	2.63
2	Ag	3.85	2.56	2.86
	Ref. 7	5.12	3.61	3.04
3	Au	4.49	3.67	1.43
	Ref. 7	5.72	4.96	1.52
4	Al	5.02	2.34	1.96
	Ref. 8	6.35	3.45	2.10
5	GaSb	3.94	3.67	1.01
	Refs. 9, 10	4.96	4.64	1.01
6	GaAs	3.65	3.44	1.11
	Ref. 11	...	...	...
7	InSb	2.76	3.08	+0.41
	Ref. 12	...	...	...
8	KCl	11.33	0.54	−0.59
	Ref. 13	13.0	1.56	−0.56
9	NaCl	9.95	0.55	0.1
	Ref. 13	11.62	1.58	0.1
10	LiF	6.78	1.55	1.0
	Ref. 13	8.18	2.60	1.0

In the alkali halides KCl, NaCl, and LiF (Ref. 13) the calculated pressure derivative of C_{11}^1 differs by a maximum value of 17% from the experimental value which is the case for LiF. The agreement between the calculated and the experimental values is poor for the pressure derivative of C_{12}^1 in the alkali halides.

The mean values of the FOEC of Cu, Ag, and Au have been computed by Hiki, Thomas, and Granato[14] using the temperature dependence of their SOEC. These estimated FOEC of Cu, Ag, and Au have been used in the present calculations to obtain the second-order anharmonic contribution to the pressure derivatives of their effective elastic constants C_{11}^1 and C_{12}^1. The contribution from FOEC to the pressure derivatives of C_{11}^1 and C_{12}^1 in Cu, Ag, and Au are reported in Table II. The deviations of the total calculated values of the pressure derivatives from their respective experimental values are due to the use of average values of the FOEC in the present work. When the second-order anharmonic contribution is taken into account, we find, as seen from Table II, that there is satisfactory agreement between

TABLE II. Contribution of FOEC to the pressure derivatives of C_{11}^1 and C_{12}^1 in Cu, Ag, and Au. The values in the brackets are the experimental values of the pressure derivatives (pressure = 10^5 bars).

Metal	Copper	Silver	Gold
(a) FOEC contribution to the pressure derivative of C_{11}^1	1.22	2.15	0.57
(b) Corrected value	5.95 (5.94)	6.00(5.12)	5.06(5.72)
(a) FOEC contribution to the pressure derivative of C_{12}^1	1.00	1.56	0.57
(b) Corrected value	4.83(5.19)	4.12(3.61)	4.24(4.96)

the calculated and the experimental pressure derivatives of the noble metals.

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Flow-enhanced corona discharge: The corona torch

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An experimental investigation has been conducted to enhance and control corona discharge in two small diameter cylindrical hollow electrodes by an external gas flow. The results show that the time-averaged corona current for fixed discharge voltages increases with increasing gas flowrate of pure nitrogen, and pressure drop is not significantly influenced by corona discharge currents.

Corona discharge is becoming an important industrial application since the recent developments in the combustion gas treatment for NO_x, CO_2, and SO_2 reductions,[1] ozonizers,[2] and in material processing.[3] In this work, an experimental investigation has been conducted to control and enhance corona discharge by an external gas flow through two small diameter cylindrical hollow electrodes (we call it "the corona torch"). Experimentally obtained time-averaged corona current-voltage characteristics as a function of gas flowrate will be discussed in detail.

The dc corona torch consists of two small diameter cylindrical hollow electrodes, as shown in Fig. 1. The gas flow enters the upstream cylindrical hollow electrode and exits at the downstream cylindrical hollow electrode. Streamer corona discharge is generated between these two electrodes. Pure nitrogen gas is introduced to the system from the bottom chamber via flow meters. The pressure drop between the bottom and the ionization chambers is measured by a Validyne model DP-15 pressure transducer. Only time-averaged corona current is reported in the present investigation.

Typical time-averaged corona current as a function of applied dc voltage for various gas flowrates is shown in Fig. 2, where the results leading in to spark or unstable discharge are not shown in this figure. Figure 2 shows that the corona current for fixed applied voltages increases with increasing gas flowrates, and also increases nearly exponentially to the applied voltages for fixed gas flowrates. Here we must note that this type of flow-enhanced corona discharge phenomena cannot be observed if electrodes are not the only flow inlet or outlet of the ionization chamber. Typical polarity effect is shown in Fig. 3, where time-averaged corona current as a function of gas flowrate for various applied voltages is shown. Figure 3 shows a significant polarity effect on the flow-enhanced corona discharges. The charge particle transport equation can be written in terms of three components, i.e., the convective terms, the drift terms, and the diffusion terms, respectively, as follows:

$$\mathbf{J} = \mathbf{U}N \pm \mu N \mathbf{E} - D\nabla N.$$

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