PERGAMON

International Journal of Non-Linear Mechanics 34 (1999) 5–11

INTERNATIONAL JOURNAL OF
NON-LINEAR MECHANICS

Apparent elastic constants of cubic crystals and their pressure derivatives

V.A. Lubarda

Department of Applied Mechanics and Engineering Sciences, University of California, San Diego, La Jolla, CA 92093-0411, USA

Received 1 August 1997, received in revised form 8 September 1997

Abstract

Expressions for the pressure-dependent apparent elastic constants of cubic crystals are derived in terms of their original second- and third-order elastic constants. New expressions are obtained for the apparent compliances and their pressure derivatives. Results are shown to be in agreement with those based on the apparent elastic moduli.

Keywords: Cubic crystals; Elastic constants; Pressure dependence

1. Introduction

Apparent second-order elastic constants appear in the relationship between the stress and strain increments from the deformed reference configuration. It is often important to know the dependence of these constants on the applied pressure. The corresponding apparent elastic moduli of cubic crystals have been calculated by several authors [1–3]. These constants appear in the relationship between the speeds of longitudinal and transverse waves in a crystal under hydrostatic and zero reference state of stress. This has been a basis for ultrasonic determination of the higher-order elastic constants [4–6], and evaluation of anharmonic properties of crystals, such as thermal expansion, Grüneisen parameters, wave mixing and attenuation, defect properties of crystals, etc. Apparent elastic constants are also important in the analysis of inelastic deformation processes under high pressures, for example in impact and penetration problems.

Previous studies reported in the literature were devoted only to apparent elastic moduli. The objective of the present study was to complete this analysis and obtain the corresponding results for the apparent elastic compliances. We have, therefore, derived the closed-form expressions for the apparent second-order elastic compliances, and their pressure derivatives, in terms of the original second- and third-order elastic compliances of cubic crystals. Obtained results are shown to be in agreement with those based on the elastic moduli approach.

2. Tensors of second- and third-order elastic constants

The strain energy per unit initial volume of an elastic solid can be expanded in a Taylor series

0020-7462/98/$19.00
PII: S0020-7462(97)00068-1

about the state of zero strain and stress as

$$\Phi = \tfrac{1}{2}C_{ijkl}E_{ij}E_{kl} + \tfrac{1}{6}C_{ijklmn}E_{ij}E_{kl}E_{mn}, \tag{1}$$

to third-order terms in the components of the Lagrangian strain E_{ij}. The Lagrangian strain is used, so that above is not effected by a superimposed rigid-body rotation of the deformed configuration. The constants C_{ijkl} and C_{ijklmn} are the second- and third-order elastic stiffness constants or elastic moduli. Since they are appropriate strain gradients of Φ evaluated at zero strain, they possess the obvious basic symmetries, such as $C_{ijklmn} = C_{jiklmn}$, and $C_{ijklmn} = C_{klijmn} = C_{mnklij}$. Tables for the second- and third-order independent elastic constants in crystals for all crystallographic groups are well known (e.g. [7]). For a cubic crystal belonging to the Laue group CI (point groups O, O_h and T_d), there are at most three independent second-oder and six independent third-order elastic constants.

The symmetric Piola–Kirchhoff stress is the gradient of the strain energy with respect to Lagrangian strain

$$S_{ij} = \frac{\partial \Phi}{\partial E_{ij}} = C_{ijkl}E_{kl} + \tfrac{1}{2}C_{ijklmn}E_{kl}E_{mn}. \tag{2}$$

The Legendre transform of Φ is the complementary strain energy $\Psi(S_{ij}) = S_{kl}E_{kl} - \Phi(E_{ij})$, which is, to within third-order terms in stress components,

$$\Psi(S_{ij}) = \tfrac{1}{2}D_{ijkl}S_{ij}S_{kl} + \tfrac{1}{6}D_{ijklmn}S_{ij}S_{kl}S_{mn}. \tag{3}$$

Thus,

$$E_{ij} = \frac{\partial \Psi}{\partial S_{ij}} = D_{ijkl}S_{kl} + \tfrac{1}{2}D_{ijklmn}S_{kl}S_{mn}\ . \tag{4}$$

The elastic constants D_{ijkl} and D_{ijklmn} are the second- and third-order elastic compliances. Since $\partial S_{ij}/\partial S_{kl} = I_{ijkl}$ (fourth-order unit tensor), and $\partial^2 S_{ij}/\partial S_{kl}\partial S_{mn} = 0$, it easily follows that the second- and third-order elastic stiffness and compliance constants are related by $D_{ijkl} = C^{-1}_{ijkl}$, and $D_{ijklmn} = -D_{ijpq}C_{pqrsuv}D_{rskl}D_{uvmn}$.

The components of the fourth-order tensor C_{ijkl} of the second-order elastic moduli of cubic crystals, with respect to an arbitrary rectangular basis, are readily found to be

$$C_{ijkl} = c_{12}\delta_{ij}\delta_{kl} + 2c_{44}I_{ijkl} + (c_{11} - c_{12} - 2c_{44})A_{ijkl}, \tag{5}$$

where

$$A_{ijkl} = a_ia_ja_ka_l + b_ib_jb_kb_l + c_ic_jc_kc_l. \tag{6}$$

In Eqs. (5) and (6), δ_{ij} denotes the Kronecker delta, while a_i, b_i and c_i are the components of the orthogonal unit vectors along the principal cubic axes. The Voigt notation $11 \sim 1$, $22 \sim 2$, $33 \sim 3$, $23 \sim 4$, $13 \sim 5$, $12 \sim 6$ is employed to relate the constants C_{ijkl} and c_{ij}. When $c_{11} - c_{12} = 2c_{44}$, C_{ijkl} are the components of isotropic fourth-order tensor, the constants c_{12} and c_{44} being the Lamé constants λ and μ. If a Cauchy symmetry $C_{ijkl} = C_{ikjl}$ applies, $c_{12} = c_{44}$.

The fourth-order tensor of the second-order elastic compliances has the components D_{ijkl} given by the right-hand side of Eq. (5), in which the constants c_{ij} are replaced by d_{ij}. The connections are

$$d_{11} = \frac{c_{11} + c_{12}}{(c_{11} - c_{12})\ (c_{11} + 2c_{12})},$$

$$d_{12} = -\frac{c_{12}}{(c_{11} - c_{12})\ (c_{11} + 2c_{12})},$$

$$d_{44} = \frac{1}{4c_{44}}. \tag{7}$$

Interchanging the symbols c and d in Eq. (7), the relationships for the second-order stiffness constants c_{ij} in terms of the second-order compliances d_{ij} are obtained. Clearly, an assumed Cauchy symmetry for the elastic moduli does not result in the corresponding symmetry for the elastic compliances. Actually, from Eq. (7) it is evident that the symmetry $D_{ijkl} = D_{ikjl}$ (i.e. $d_{12} = d_{44}$) is out of question for all cubic crystals with positive c_{12}, since then d_{12} is negative, while d_{44} is always positive. Recall that the Born stability condition requires $c_{11} + 2c_{12} > 0$, $c_{11} - c_{12} > 0$, and $c_{44} > 0$. A comprehensive review of some fundamental problems in crystal elasticity has been given in [8].

The components of the sixth-order tensor C_{ijklmn} of the third-order elastic moduli of cubic crystals, with respect to an arbitrary rectangular basis, can be written as [9]

$$C_{ijklmn} = \gamma_1\delta_{ij}\delta_{kl}\delta_{mn} + \gamma_2\delta_{(ij}I_{klmn)} + \gamma_3\delta_{(ik}\delta_{lm}\delta_{nj)} + \gamma_4\delta_{(ij}A_{klmn)} + \gamma_5 a_{(i}a_jb_kb_lc_mc_{n)} + \gamma_6 a_{(i}b_jc_ka_lb_mc_{n)}. \tag{8}$$

The following abbreviations were used:

$$\gamma_1 = c_{123} - \beta_5, \quad \gamma_2 = 6c_{144}, \quad \gamma_3 = 2\beta_3,$$
$$\gamma_4 = -3\beta_4, \quad \gamma_5 = 6\beta_5, \quad \gamma_6 = 6\beta_6. \tag{9}$$

The coefficients β_1–β_6 are defined by

$$\beta_1 = \tfrac{1}{6}c_{111}, \quad \beta_2 = -2c_{244}, \quad \beta_3 = 2(c_{244} - c_{144}),$$
$$\beta_4 = \tfrac{1}{2}(c_{112} - c_{111} + 4c_{244}),$$
$$\beta_5 = \tfrac{1}{2}(c_{111} - 3c_{112} + 2c_{123} + 4c_{144} - 4c_{244}),$$
$$\beta_6 = 4(c_{144} - c_{244} + 2c_{456}). \tag{10}$$

The tensors appearing on the right-hand side of Eq. (8) are the base tensors for the sixth-order elastic moduli tensor with cubic symmetry. The notation such as $a_{(i}a_jb_kb_lc_mc_{n)}$ designates the symmetrization with respect to i and j, k and l, m and n, and ij, kl and mn. Other base tensors could be selected, such as those used in [10]. For instance, it can be shown that

$$A_{ijklmn} = a_ia_ja_ka_la_ma_n + b_ib_jb_kb_lb_mb_n + c_ic_jc_kc_lc_mc_n$$
$$= \tfrac{1}{2}[-\delta_{ij}\delta_{kl}\delta_{mn} + 3\delta_{(ij}A_{klmn)} + 6a_{(i}a_jb_kb_lc_mc_{n)}]. \tag{11}$$

In the case of isotropy, $\beta_4 = \beta_5 = \beta_6 = 0$, i.e. $c_{111} = c_{123} + 6c_{144} + 8c_{456}$, $c_{112} = c_{123} + 2c_{144}$, and $c_{244} = c_{144} + 2c_{456}$. The components C_{ijklmn} are then the components of an isotropic sixth-order tensor

$$C_{ijklmn} = c_{123}\delta_{ij}\delta_{kl}\delta_{mn} + 6c_{144}\delta_{(ij}I_{klmn)}$$
$$+ 8c_{456}\delta_{(ik}\delta_{lm}\delta_{nj)}. \tag{12}$$

If a Cauchy type or Milder symmetry $C_{ijklmn} = C_{ikjlmn}$ is assumed, then $c_{123} = c_{144} = c_{456}$. The three independent third-order elastic constants of an isotropic material (c_{123}, c_{244} and c_{456}) are related to Murnaghan's [11] constants l, m and n by $l = c_{144} + c_{123}/2$, $m = c_{144} + 2c_{456}$, and $n = 4c_{456}$. Toupin and Bernstein [5] used the notation $v_1 = c_{123}$, $v_2 = c_{144}$ and $v_3 = c_{456}$, referring to them as the third-order Lamé constants.

The components of the sixth-order elastic compliance tensor D_{ijklmn} are exactly the same as those given by Eq. (8), with the constants c_{ijk} replaced by d_{ijk} in Eqs. (9) and (10).

Having in mind that $d_{ikm} = -d_{ip}c_{pru}d_{rk}d_{um}$, and in view of tables for independent second- and third-order elastic constants given in [7], the relationships between the third-order elastic moduli and compliances are

$$d_{111} = -(d_{11}^3 + 2d_{12}^3)c_{111}$$
$$- 6d_{12}(d_{11}^2 + d_{11}d_{12} + d_{12}^2)c_{112}$$
$$- 6d_{11}d_{12}^2c_{123}, \tag{13}$$

$$d_{112} = -d_{12}(d_{11}^2 + d_{11}d_{12} + d_{12}^2)(c_{111} + 2c_{123})$$
$$- (d_{11}^3 + 3d_{11}^2d_{12} + 9d_{11}d_{12}^2 + 5d_{12}^3)c_{112}, \tag{14}$$

$$d_{123} = -3d_{11}d_{12}^2c_{111}$$
$$- 6d_{12}(d_{11}^2 + d_{11}d_{12} + d_{12}^2)c_{112}$$
$$- (d_{11}^3 + 3d_{11}d_{12}^2 + 2d_{12}^3)c_{123}, \tag{15}$$

$$d_{144} = -4d_{44}^2(d_{11}c_{144} + 2d_{12}c_{244}), \tag{16}$$

$$d_{244} = -4d_{44}^2[d_{12}c_{144} + (d_{11} + d_{12})c_{244}], \tag{17}$$

$$d_{456} = -8d_{44}^3c_{456}. \tag{18}$$

If the symbols c and d are interchanged in Eqs. (13)–(18), the inverse relationships, expressing c_{ijk} in terms of d_{ijk}, are obtained.

3. Apparent elastic constants and their pressure derivatives

The apparent second-order elastic constants play an important role in the calculation of the third-order elastic constants. Their pressure derivatives appear in the relationship between the speeds of longitudinal and transverse waves in the body under hydrostatic and zero reference state of stress. They can be used to determine the volume expansion of self-strained isotropic elastic body, since the average dilatation is dependent on the pressure derivatives of the second-order bulk and shear moduli. The apparent elastic constants are also of importance in modeling inelastic deformation under high pressures, to more accurately express elastic part of the total strain increment in terms of an applied stress increment.

For the sake of comparison with the new results presented for the apparent elastic compliances in Section 3.2, we begin this section with the derivation of relevant results for the apparent elastic moduli of cubic crystals.

3.1. Apparent elastic moduli

If a hydrostatic pressure p is applied to an unstressed configuration of a cubic crystal, the resulting deformation gradient is $\mathbf{F}_\vartheta = \vartheta \mathbf{I}$, $0 < \vartheta \leqslant 1$. (An analogous derivation proceeds in the case of hydrostatic tension, when $\vartheta \geqslant 1$.) If an additional stress is subsequently applied, which produces infinitesimal elastic strain ε_{ij} and rotation ω_{ij}, the corresponding deformation gradient is $\mathbf{F}_\varepsilon = \mathbf{I} + \nabla \mathbf{u}$, where $\mathbf{u}$ is the infinitesimal displacement relative to the compressed configuration. The total deformation gradient is $\mathbf{F} = \mathbf{F}_\varepsilon \mathbf{F}_\vartheta = \vartheta(\mathbf{I} + \nabla \mathbf{u})$, and the Lagrangian strain components are

$$E_{ij} = e\delta_{ij} + \vartheta^2 \varepsilon_{ij}, \quad e = \tfrac{1}{2}(\vartheta^2 - 1). \tag{19}$$

Substituting this into Eq. (2), we obtain

$$S_{ij} = \tfrac{1}{3}(eC_{ppqq} + \tfrac{1}{2}e^2 C_{ppqqrr})\delta_{ij} + \vartheta^2(C_{ijkl} + eC_{ijklmm})\varepsilon_{kl}, \tag{20}$$

neglecting quadratic and higher-order terms in ε.

The Cauchy stress σ is related to symmetric Piola–Kirchhoff stress $\mathbf{S}$ by $\sigma = (\det \mathbf{F})^{-1}\mathbf{F}\mathbf{S}\mathbf{F}^{\mathrm{T}}$. Thus, in view of the expression for the deformation gradient $\mathbf{F}$,

$$\sigma_{ij} = \frac{1}{\vartheta}(S_{ij} - \varepsilon_{kk}S_{ij} + \varepsilon_{ik}S_{kj} + S_{ik}\varepsilon_{kj} + \omega_{ik}S_{kj} - S_{ik}\omega_{kj}). \tag{21}$$

The quadratic terms in displacement gradient were neglected.

In a hydrostatically compressed configuration, $\mathbf{F} = \mathbf{F}_\vartheta = \vartheta \mathbf{I}$, and $\sigma = -p\mathbf{I} = \mathbf{S}/\vartheta$. From Eq. (20) it, consequently, follows that

$$p = -\frac{1}{3\vartheta}(eC_{iijj} + \frac{1}{2}e^2 C_{iijjkk}), \tag{22}$$

which defines a pressure/volume relation for the cubic crystal. Substitution of Eq. (20) into Eq. (21), therefore, gives

$$\sigma_{ij} = -p\delta_{ij} + [\vartheta(C_{ijkl} + eC_{ijklmm}) + p(\delta_{ij}\delta_{kl} - 2I_{ijkl})]\varepsilon_{kl}, \tag{23}$$

to within linear terms in ε.

On the other hand, the stress–strain response from a hydrostatically compressed configuration can be written as

$$\sigma_{ij} = -p\delta_{ij} + C^{(p)}_{ijkl}\varepsilon_{kl}, \tag{24}$$

where $C^{(p)}_{ijkl}$ are the apparent second-order elastic moduli in the compressed configuration. Comparison of Eqs. (23) and (24) finally yields

$$C^{(p)}_{ijkl} = \vartheta(C_{ijkl} + eC_{ijklmm}) + p(\delta_{ij}\delta_{kl} - 2I_{ijkl}), \tag{25}$$

which defines the pressure-dependent apparent elastic moduli $C^{(p)}_{ijkl}$ of a cubic crystal. The terminology "current elastic moduli" is also used. These moduli appear in the linearized equations of motion for the small displacements u_i from the hydrostatically compressed reference state with density ρ, i.e. $C^{(p)}_{ijkl}u_{k,jl} = \rho \ddot{u}_i$. (Recall that displacement gradients are also small.) The corresponding acoustic tensor, whose eigenvectors are the polarization directions and eigenvalues the wave speeds, is $C^{(p)}_{ijkl}n_j n_l$, where n_j are the components of the wave propagation direction. The moduli $C^{(p)}_{ijkl}$ in the reference configuration under pressure p possess full symmetry. This is not the case for the apparent moduli in the reference configuration under non-hydrostatic state of stress, when additional five deviatoric stress components make $C^{(p)}_{ijkl}$ (slightly) anisotropic, even for an initially isotropic material (stress-induced anisotropy). Furthermore, if a Cauchy symmetry applies for the moduli C_{ijkl} and C_{ijklmn} ($c_{12} = c_{44}$, $c_{112} = c_{244}$, $c_{123} = c_{144} = c_{456}$), from Eq. (25) it is evident that the moduli $C^{(p)}_{ijkl}$ do not obey such symmetry, since $c^{(p)}_{12} - c^{(p)}_{44} = p$.

Differentiating Eq. (25) with respect to pressure p, and evaluating the result at zero pressure, gives

$$\left[\frac{\partial C^{(p)}_{ijkl}}{\partial p}\right]_0 = -\frac{1}{3\kappa}(C_{ijkl} + C_{ijklmm}) + \delta_{ij}\delta_{kl} - 2I_{ijkl}, \tag{26}$$

where $\kappa = C_{iijj}/9 = (c_{11} + 2c_{12})/3$ is the bulk modulus at zero pressure. This equation was originally obtained through a thermodynamic analysis by Barsch [3], although its component by component form was previously derived by Birch [1]; see also [12].

From Eq. (26), we have

$$\left[\frac{\partial \kappa^{(p)}}{\partial p}\right]_0 = -\frac{1}{27\kappa}C_{iijjkk} = -\frac{1}{9\kappa}(c_{111} + 6c_{112} + 2c_{123}). \tag{27}$$

Derivative of the constant $C^{(p)}_{2323} = c^{(p)}_{44}$ is likewise

$$\left[\frac{\partial c^{(p)}_{44}}{\partial p}\right]_0 = -\frac{1}{3\kappa}(c_{44} + c_{144} + 2c_{244}) - 1. \tag{28}$$

If a longitudinal wave is propagating along a pure mode direction **n**, the corresponding wave speed is obtained from $\rho v^2 = C^{(p)}_{ijkl}n_i n_j n_k n_l$. Thus, if ρ_0 is the initial density in the undeformed state, and v_0 is the corresponding wave speed, we have to within a linear approximation [5]

$$\rho v^2 - \rho_0 v_0^2 = p\left[\frac{\partial C^{(p)}_{ijkl}}{\partial p}\right]_0 n_i n_j n_k n_l. \tag{29}$$

Thurston and Brugger [6] derived expressions for arbitrary crystal symmetry, and for any reference homogeneous stress state depending on a single parameter. Implications of the symmetry conditions for the third-order elastic constants in the non-linear wave theory have been recently discussed in [13]. There has also been a significant amount of research devoted to higher-order elastic constants from the molecular dynamics point of view, and assumed structure of the potential energy between two atoms [14].

3.2. Apparent elastic compliances

In a dual approach to that described in the previous subsection, we introduce the apparent elastic compliances $D^{(p)}_{ijkl}$, so that, relative to hydrostatically compressed configuration,

$$\varepsilon_{ij} = D^{(p)}_{ijkl}t_{kl}, \quad t_{kl} = \sigma_{kl} + p\delta_{kl}. \tag{30}$$

In order to derive an expression for $D^{(p)}_{ijkl}$, we first have from the relationship between the Piola–Kirchhoff and Cauchy stress,

$$S_{ij} = \vartheta(t_{ij} - p\delta_{ij} - p\varepsilon_{kk}\delta_{ij} + 2p\varepsilon_{ij}). \tag{31}$$

Substitution of Eq. (31) into Eq. (4) gives

$$\begin{aligned} E_{ij} = {} & \vartheta(D_{ijkl} - \vartheta p D_{ijklmm})t_{kl} \\ & - \tfrac{1}{3}\vartheta(pD_{ppqq} - \tfrac{1}{2}\vartheta p^2 D_{ppqqrr})\,\delta_{ij} \\ & + [2\vartheta p(D_{ijkl} - \tfrac{1}{6}D_{ppqq}\delta_{ij}\delta_{kl}) \\ & - 2\vartheta^2 p^2(D_{ijklmm} - \tfrac{1}{6}D_{ppqqrr}\delta_{ij}\delta_{kl})]\varepsilon_{kl}, \end{aligned} \tag{32}$$

to within linear terms in ε. Comparison of Eqs. (19) and (32), therefore, yields

$$e = -\tfrac{1}{3}\vartheta(pD_{iijj} - \tfrac{1}{2}\vartheta p^2 D_{iijjkk}), \tag{33}$$

and

$$\begin{aligned} & \left[I_{ijkl} - \frac{2p}{\vartheta}\left(D_{ijkl} - \frac{1}{6}D_{ppqq}\delta_{ij}\delta_{kl}\right)\right. \\ & \quad \left. + 2p^2\left(D_{ijklmm} - \frac{1}{6}D_{ppqqrr}\delta_{ij}\delta_{kl}\right)\right]\varepsilon_{kl} \\ & \quad = \frac{1}{\vartheta}(D_{ijkl} - \vartheta p D_{ijklmm})t_{kl}. \end{aligned} \tag{34}$$

Eq. (33) is a dual equation to Eq. (22). It gives a pressure/volume relation associated with the second-order approximation in the constitutive expression of Eq. (4). Observe that Eqs. (22) and (33) are equivalent only to within the second-order terms in e, because the cubic approximations of the strain and complementary energies are not exactly the Legendre transforms of each other.

Inversion of Eq. (34) gives, to the same order of approximation,

$$\begin{aligned} \varepsilon_{ij} = {} & \frac{1}{\vartheta}\left[I_{ijkl} + \frac{2p}{\vartheta}\left(D_{ijkl} - \frac{1}{6}D_{ppqq}\delta_{ij}\delta_{kl}\right)\right. \\ & \left. - 2p^2\left(D_{ijklmm} - \frac{1}{6}D_{ppqqrr}\delta_{ij}\delta_{kl}\right)\right] \\ & \times (D_{ijkl} - \vartheta p D_{ijklmm})t_{kl}. \end{aligned} \tag{35}$$

This can be regrouped into

$$\varepsilon_{ij} = \left[\frac{1}{\vartheta}(D_{ijkl} - \vartheta p D_{ijklmm}) + \frac{2p}{\vartheta^2} D_{ijmn} D_{klmn} - \frac{p}{9\vartheta^2}(D_{ppqq} - \vartheta p D_{ppqqrr})^2 \delta_{ij}\delta_{kl} - 2\frac{p^2}{\vartheta}(D_{ijmn} D_{klmnpp} + D_{klmn} D_{ijmnpp}) + 2p^3 D_{ijmnpp} D_{klmnqq} \right] t_{kl}. \quad (36)$$

Comparison of Eq. (36) and the first part of Eq. (30), therefore, gives

$$D^{(p)}_{ijkl} = \frac{1}{\vartheta}(D_{ijkl} - \vartheta p D_{ijklmm}) + \frac{2p}{\vartheta^2} D_{ijmn} D_{klmn} - \frac{p}{9\vartheta^2}(D_{ppqq} - \vartheta p D_{ppqqrr})^2 \delta_{ij}\delta_{kl} - 2\frac{p^2}{\vartheta}(D_{ijmn} D_{klmnpp} + D_{klmn} D_{ijmnpp}) + 2p^3 D_{ijmnpp} D_{klmnqq}. \quad (37)$$

This represents the pressure dependent apparent elastic compliances of cubic crystals, relative to a hydrostatically compressed reference configuration. These compliances evidently possess the full symmetry $D^{(p)}_{klij} = D^{(p)}_{ijkl} = D^{(p)}_{jikl}$.

Derivative of Eq. (37) with respect to pressure p, evaluated at zero pressure, is

$$\left[\frac{\partial D^{(p)}_{ijkl}}{\partial p} \right]_0 = \frac{1}{3} k D_{ijkl} - D_{ijklmm} + 2 D_{ijmn} D_{klmn} - \frac{1}{9} k^2 \delta_{ij}\delta_{kl}, \quad (38)$$

where $k = D_{iijj} = 3(d_{11} + 2d_{12})$ is the compressibility constant at zero pressure ($k = 1/\kappa$).

Eq. (38) is a dual equation to Eq. (26). To our knowledge, it has not been previously reported in the literature. This is presumably because more interest was placed on the pressure derivatives of apparent elastic moduli, due to their direct use in the structure of the wave equation. Equation (38) is, however, of significance for determination of the third-order elastic compliances, whenever the values of pressure dependent apparent elastic compliances are experimentally reported. For example, from Eq. (38) it follows that

$$\left[\frac{\partial k^{(p)}}{\partial p} \right]_0 = -D_{iijjkk} = -3(d_{111} + 6d_{112} + 2d_{123}). \quad (39)$$

This is in agreement with Eq. (27), because $C_{iijjkk} = -27\kappa^3 D_{iijjkk}$. Derivative of the constant $D^{(p)}_{2323} = d^{(p)}_{44}$ is similarly found to be

$$\left[\frac{\partial d^{(p)}_{44}}{\partial p} \right]_0 = \frac{1}{3} k d_{44} + 4d_{44}^2 - (d_{144} + 2d_{244}). \quad (40)$$

In view of Eqs. (7), (16) and (17) it is readily verified that Eq. (40) is also in agreement with the corresponding Eq. (28), obtained in the analysis based on the apparent elastic moduli.

Acknowledgements

Research support provided by the Alcoa Center and discussions with Dr. Owen Richmond are kindly acknowledged.

References

[1] F. Birch, Finite elastic strain of cubic crystals, Phys. Rev. 71 (1947) 809.

[2] G. Leibfried, W. Ludwig, Theory of anharmonic effects in crystals, Solid State Phys. 12 (1961) 275.

[3] G.R. Barsch, Adiabatic, isothermal, and intermediate pressure derivatives of the elastic constants for cubic symmetry, Phys. Stat. Sol. 19 (1967) 129.

[4] W.B. Daniels, C.S. Smith, Pressure derivatives of the elastic constants of copper, silver, and gold to 10,000 bars, Phys. Rev. 111 (1958) 713.

[5] R.A. Toupin, B. Bernstein, Sound waves in deformed perfectly elastic materials. Acoustoelastic effect, J. Acoust. Soc. Amer. 33 (1961) 216.

[6] R. N. Thurston, K. Brugger, Third-order constants and the velocity of small amplitude elastic waves in homogeneously stressed media, Phys. Rev. 133 (1964) A1604.

[7] K. Brugger, Pure modes for elastic waves in crystals, J. Appl. Phys. 36 (1965) 759.

[8] F. Milstein, Crystal elasticity, in: H.G. Hopkins, M.J. Sewell (Eds.), Mechanics of Solids—The Rodney Hill 60th Anniversary Volume, Pergamon Press, Oxford, 1982, pp. 417–452.

[9] V.A. Lubarda, New estimates of the third-order elastic constants for isotropic aggregates of cubic crystals, J. Mech. Phys. Solids 45 (1997) 471.

[10] R.A. Toupin, R.S. Rivlin, Dimensional changes in crystals caused by dislocations, J. Math. Phys. 1 (1960) 8.
[11] F.D. Murnaghan, Finite Deformation of an Elastic Solid, Wiley, New York, 1951.
[12] D.H. Chung, First pressure-derivatives of polycrystalline elastic moduli: Their relation to single-crystal acoustic data and thermodynamic relations, J. Appl. Phys. 38 (1967) 5104.
[13] A.N. Norris, Symmetry conditions for third order elastic moduli and implications in non-linear wave theory, J. Elasticity 25 (1991) 247.
[14] T. Çağin, B.M. Pettitt, Elastic constants of nickel: Variations with respect to temperature and pressure, Phys. Rev. B 39 (1989) 12484.