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THE ELASTIC CONSTANTS OF A CUBIC CRYSTAL SUBJECTED TO MODERATELY HIGH HYDROSTATIC PRESSURE

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Abstract—This paper presents the results of an analysis of the finite strain theory that goes to the next higher-order term than third-order in the strains for cubic crystals. Theoretical expressions for the effective second-order elastic constants are presented here in terms of the second-, third-, and fourth-order elastic constants and the Lagrangian strain; these have been derived from the rigorous stress-strain relationship set by the Murnaghan theory of finite deformation. Since typical ultrasonic experiments with pressure result in *thermodynamically mixed* elastic constants, the practical ultrasonic expressions of the effective elastic constants are presented for a cubic crystal subjected to moderately high hydrostatic compression. The rigorous relationships between the pressure derivatives of the effective elastic constants and partial contractions of the higher-order elastic constants are presented also, and then the primary experimental quantities that are resulting from the usual ultrasonic-pressure experiments have been identified in terms of the *thermodynamically mixed* second-, third-, and fourth-order elastic constants of the crystal.

1. INTRODUCTION

THE FINITE strain theory for a medium of the cubic symmetry subjected to a finite hydrostatic compression was first developed by Birch[1]. In this work, Birch had defined the free-energy of a crystal in terms of a power series of the energy in the strain components including terms up to the third-order in the strains and then derived expressions for the effective elastic constants of the crystal under hydrostatic pressure. These expressions contained the second- and third-order elastic constants of crystal, and they were shown to describe the effective elastic properties of cubic crystals subjected to relatively 'low' compression.* For a crystal subjected to moderately 'high' compression, however, the higher order terms than the third-order in the strains would play an important role in the description of crystal elasticity under this high pressure.

This paper presents the results of our analysis of the finite strain theory that goes to the next higher order term than the third-order in the strains for cubic crystals. In the following, expressions for the effective elastic constants resulting from the rigorous stress-strain relationship set by the Murnaghan theory of finite deformation[2] will be presented and compared with the earlier work. Since typical ultrasonic experiments with pressure result in *thermodynamically mixed* elastic constants, the derived expressions of the effective elastic constants had to be identified according to their thermodynamic boundary conditions. This is done in Section 3. In Section 4, we present the rigorous relation of pressure derivatives of the effective elastic constants to partial contractions of the higher-order elastic constants. And, in Section 5, the present work is summarized with a brief discussion.

2. THE EFFECTIVE ELASTIC CONSTANTS

Using the usual Cartesian coordinates, we take the principal axes to coincide with the symmetry axes of an unstrained cubic crystal. Let us denote the coordinates of a point p in the crystal before strain by (a_1, a_2, a_3) and

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*The terms 'low' and 'high' compressions as used here are meant to imply the following: For a given solid under hydrostatic pressure, if the change in the second-order elastic constants with pressure is *linear*, this pressure (and up to this pressure) is referred to as relatively 'low' pressure. If the change with pressure is *nonlinear*, the pressures higher than this pressure are referred to as relatively 'high' pressure. Although it is difficult to make a sharp boundary between the 'low' and 'high' pressures, the pressure in the order of 0·05 B^T (where B^T is the isothermal bulk modulus of solid under the study) for most solids can be referred to as the *relatively low* pressure and the pressure in the order of 0·1 B^T may be referred to as the *moderately high* pressure.

those in the crystal after a strain by (x_1, x_2, x_3). These points determine then a displacement vector with components $(x-a_1)$, (x_2-a_2), (x_3-a_3); thus, the components of the displacements are simply

$$u_r = x_r - a_r, \quad (r = 1, 2, 3). \tag{1}$$

For this reason, it is convenient to discuss the strain according to the Lagrangian scheme.

The Lagrangian strain components in Murnaghan's notation are[2]

$$\eta_{rs} = \tfrac{1}{2}\left(\frac{\partial x_p}{\partial a_r} \cdot \frac{\partial x_p}{\partial a_s} - \delta_{rs}\right) \tag{2}$$

where the subscripts ranges are 1, 2, 3 and δ_{rs} are the Kronecker deltas. Using the Jacobian J of the deformation, we can write equation (2) in a compact form as

$$[\eta] = \tfrac{1}{2}(J^*J - I_3) \tag{2a}$$

where J^* is the transpose of J given by

$$J = \frac{\partial(x_1, x_2, x_3)}{\partial(a_1, a_2, a_3)} \tag{3}$$

and I_3 is the unit matrix.

Consider a special strain which is composed of a hydrostatic strain and a subsequent homogeneous strain. By the homogeneous strain, the point p initially at (a_1, a_2, a_3) is brought to the point $(x_1{}^0, x_2{}^0, x_3{}^0)$, given by

$$x_s{}^0 = (1-\alpha)a_s, \quad (s = 1, 2, 3) \tag{4}$$

thus, every line in the crystal is shortened by the factor $(1-\alpha)$, where

$$\alpha \equiv \eta(\tfrac{1}{2}\eta - 1). \tag{5}$$

The additional displacements resulting from the homogeneous strain are then

$$u'_r = \sum_s \beta_{rs} x_s{}^0, \quad (r, s = 1, 2, 3) \tag{6}$$

where $\beta_{rs} = \beta_{sr}$; thus, β_{rs} represent the six homogeneous strain components and they are infinitesimal quantities. The final coordinates are then given by

$$x_r = x_r{}^\circ + u'_r. \tag{7}$$

From these, we find that

$$\frac{\partial x_r}{\partial a_s} = (1-\alpha)(\delta_{rs} + \beta_{rs}). \tag{8}$$

Here, since β_{rs} are infinitesimal quantities as noted above, only the first powers of β_{rs} are retained and all others are neglected. In view of the particular strain defined by equation (7), the Lagrangian strains become

$$\eta_{rs} = \delta_{rs}\eta + \beta_{rs}(1+2\eta). \tag{9}$$

The strain energy density Φ per unit initial volume is usually given by a power series of the Lagrangian strains as

$$\Phi = \phi_0 + \phi_1 + \phi_2 + \phi_3 + \phi_4 + \ldots \tag{10}$$

where ϕ_j contains the jth order terms of η_{ij} and for a body with no initial stresses ϕ_0 and ϕ_1 can be set equal to zero. Thus, ϕ_2, ϕ_3, and ϕ_4 are:

$$\phi_2 = \frac{1}{2!} C_{ijkl}\eta_{ij}\eta_{kl}$$

and

$$\phi_3 = \frac{1}{3!} C_{ijklmn}\eta_{ij}\eta_{kl}\eta_{mn} \tag{11}$$

$$\phi_4 = \frac{1}{4!} C_{ijklmnop}\eta_{ij}\eta_{kl}\eta_{mn}\eta_{op}$$

where the subscripts ranges are 1, 2, 3 and the Einstein summation convention for repeated subscripts is assumed. The rigorous relation of the stresses T_{rs} to the strains η_{pq} is

$$T_{rs} = \left(\frac{\rho}{\rho_0}\right)\frac{\partial x_r}{\partial a_p}\left[\frac{\partial \Phi}{\partial \eta_{pq}}\right]\frac{\partial x_s}{\partial a_q} \tag{12}$$

or in a compact form

$$[T] = \left(\frac{\rho}{\rho_0}\right)J\left[\frac{\partial \Phi}{\partial \eta}\right]J^*. \tag{12a}$$

Here, ρ_0 and ρ are the crystal densities before and after a strain, respectively, and the compression ratio is

$$\left(\frac{\rho}{\rho_0}\right) = \frac{1}{\det J} \tag{13}$$

and the gradient of Φ with respect to η_{pq} is

$$\frac{\partial \Phi}{\partial \eta_{pq}} = \left\{\begin{matrix} \dfrac{\partial \Phi}{\partial \eta_{11}} & \dfrac{\partial \Phi}{\partial \eta_{12}} & \dfrac{\partial \Phi}{\partial \eta_{13}} \\ \dfrac{\partial \Phi}{\partial \eta_{21}} & \dfrac{\partial \Phi}{\partial \eta_{22}} & \dfrac{\partial \Phi}{\partial \eta_{23}} \\ \dfrac{\partial \Phi}{\partial \eta_{31}} & \dfrac{\partial \Phi}{\partial \eta_{32}} & \dfrac{\partial \Phi}{\partial \eta_{33}} \end{matrix}\right\} \tag{14}$$

From this relation (12), as was done by Birch[1], we can set

$$T_{rs} = -P\delta_{rs} + T'_{rs} \tag{15}$$

where $-P$ is hydrostatic pressure given by

$$-P = \frac{1}{1-\alpha}\left(\frac{\partial \Phi^{(0)}}{\partial \eta_{11}}\right) \tag{16}$$

and T'_{rs} are expressed in terms of the β's and '*a new set*' of elastic constants. This new set of the elastic constants are the effective second-order elastic constants under the hydrostatic pressure and we will denote hereafter to as C_{11}, C_{12} and C_{44}. Since

$$T'_{11} = C_{11}\beta_{11} + C_{12}(\beta_{22} + \beta_{33}) \tag{17}$$