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Iterative Procedure to Estimate the Values of Elastic Constants of a Cubic Solid at High Pressures from the Sound Wave Velocity Measurements

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In order to estimate accurately the values of the elastic constants of a solid at high pressure and at an arbitrary temperature T from the ultrasonic measurements of the velocities of elastic waves propagated in solids as a function of pressure at the temperature T, it is necessary to know *a priori* the compressibility of the solid as a function of pressure at the temperature T. However, this latter information is not always available. Hence, one has to make some kind of approximation to estimate the values of the elastic constants of solids at high pressure. The procedure developed here is more consistent than previous procedures. It requires *a priori* knowledge of the following values: the thermal expansion coefficient, its temperature derivative, the specific heat at constant pressure of a solid at one atmosphere, and the travel-time measurements of the elastic waves propagated through the solid as a function of pressure at a temperature T or at more than one temperature.

INTRODUCTION

An investigator attempting to determine the variation of elastic constants of solids with pressure by ultrasonic measurements on new (or even well known) materials may find that the needed compressibility measurements are either unavailable or if available are unreliable. Cook's method enables one to obtain an estimate of the values of the elastic constants of a solid at high pressure without *a priori* knowledge of the compressibility of the substance.[1] In developing the estimating procedure Cook assumed that the parameter $\Delta(P)$ [c.f. General Notation and Analysis Section, Eq. (5)], remained constant with pressure. The value of $\Delta(P)$ at any pressure P is given by its magnitude at one atmosphere. Ruoff[2] extended the results of Cook in the case of cubic solids by presenting an estimating procedure which permitted the parameter $\Delta(P)$ to vary with pressure. This was done by expressing $\Delta(P)$ in a power series expansion given by (1):

$$\Delta(P)=\Delta(P=1)+P[\partial\Delta(P)/\partial P]_{P\to1}+\tfrac{1}{2}P^2[\partial^2\Delta(P)/\partial P^2]_{P\to1}+\cdots, \quad (1)$$

where the quantities on the right-hand side of (1) are evaluated at 1 atm.

Even so the lack of relevant data in the case of most materials limits one to the first derivative of $\Delta(P)$. This is easily seen by differentiating $\Delta(P)$ with respect to pressure P. The present work develops an iterative procedure to estimate the values of the elastic constants of cubic solids at high pressure which differs from the one developed by Ruoff with respect to the assumptions regarding (i) the pressure derivative of the thermal volume expansion coefficient at a temperature T, (ii) the temperature derivative of the volume thermal expansion coefficient at a pressure P, and (iii) the estimation procedure for $\Delta(P)$. It is shown here that no assumptions regarding (i) and (ii) are necessary in order to estimate the elastic constants of cubic solids at higher pressures provided the ultrasonic measurements are made as a function of pressure at more than one temperature. This enables one to compute a more realistic estimate of elastic constants of cubic solids as a function of pressure.

The size, density, and elastic constants of a material specimen change with the application of pressure. The concomitant changes are observed in the value of the resonant or null frequencies of a standing wave and also in the measurement of travel-time for a pulse between flat parallel faces of the specimen. The analysis presented in this paper refers to frequency measurements but is equally valid for the travel-time measurements of an elastic wave propagated in a medium.

GENERAL NOTATION AND ANALYSIS

By a solid we always refer to a cubic solid. Even though the quantities dealt with here refer to a pressure P and a temperature T, for simplicity the relevant suffix for the temperature is dropped from the general notation.

$\rho(P)$	the density of the material at pressure P
$\beta(P)$	volume-expansion coefficient of the material at pressure P
$C_P(P)$	specific heat at constant-pressure of the material at pressure P
$B^S(P)$	adiabatic bulk modulus of the material at pressure P
$B^T(P)$	isothermal bulk modulus of the material at pressure P
$\chi^T(P)$	isothermal compressibility of the material at pressure P
$L(J, P)$	the thickness of the specimen used in the measurement of the Jth velocity mode at pressure P
$\lambda(P)$	$=L(J, P_1)/L(J, P)$; $P_1<P$; $P=1=$ 1 atm or 1 bar, only in the case of cubic material

$V(J, P)$	the Jth velocity mode in the material at pressure P
$\tau(J, P)$	the travel-time for the Jth velocity mode at pressure P
$F(I, J, P)$	the Ith null frequency observed for the Jth velocity mode in the material at pressure P
$N(I, J, P)$	the number of $\frac{1}{2}$ wavelengths in the specimen corresponding to $F(I, J, P)$
$\tau(I, J, P)$	the travel time in the specimen corresponding to $F(I, J, P)$
$IMP(J, P)$	mechanical impedance of quartz transducer for Jth velocity mode at pressure P
$K(I, J, P)$	$IMP(J, P)$/(mechanical impedance of the material corresponding to $\tau(I, J, P)$
$V(1, P)$	longitudinal velocity in the (100) direction at pressure P
$V(2, P)$	shear velocity in the (100) directtion a pressure P
$V(3, P)$	longitudinal velocity in the (110) direction at pressure P

We need only know any three independent velocity modes in order to obtain the three elastic constants of a solid. In this paper the resonant frequencies measured as a function of pressure for the longitudinal modes of propagation in the (100) and (110) directions and the shear mode of propagation in the (100) direction have been used.[3]

We also assume the following:

(i) The temperature dependence of the volume, or the linear expansion coefficient at a temperature T and one atmosphere is known;

(ii) the specific heat at temperature T and one atmosphere is known; and

(iii) $[\partial\beta(P)/\partial T]_P \simeq [\partial\beta(P_1)/\partial T]_{P_1}$, where $P \geq P_1$, holds.[4]

Then the procedure outlined below can be used to estimate the elastic constants of solids at higher pressures, without reference to *a priori* knowledge of the compressibility of the substance.

The relation between the adiabatic bulk modulus and $V^2(J, P)$, $(J=1, 3)$, in a cubic solid may be written as

$$B^S(P) = \tfrac{1}{3}\rho(P)[4V^2(3, P) - 4V^2(2, P) - V^2(1, P)]. \quad (2)$$

Relation (1), expressed in terms of $L(J, P_1)$, $\tau(J, P)$, $\lambda(P)$, and $\rho(P_1)$, is given as relation (3):

$$B^S(P) = \tfrac{1}{3}\rho(P_1)\lambda(P)[4L^2(3, P_1)/\tau^2(3, P) - 4L^2(2, P_1)/\tau^2(2, P) - L^2(1, P_1)/\tau^2(1, P)], \quad (3)$$

where $\rho(P) = \lambda^3(P)\rho(P_1)$. By the definition of isothermal bulk modulus we obtain

$$B^T(P) = -\text{Vol.}(P)[\partial P/\partial\,\text{Vol.}(P)]_T = \rho(P)[\partial P/\partial\rho(P)]_T = \tfrac{1}{3}\lambda(P)[\partial P/\partial\lambda(P)]_T. \quad (4)$$

And if

$$\Delta(P) = \beta^2(P)B^S(P)T/\rho(P)C_P(P) \quad (5)$$

where temperature T is in Kelvin, then

$$B^T(P) = B^S(P)/[1+\Delta(P)]. \quad (6)$$

Using Williams and Lamb's[5] method of ultrasonic wave velocity measurements as modified by Colvin,[6] transit time for the various wave propagations is obtained from the following relations:

$$N(I, J, P) = \text{Integer}\{[F(I, J, P)/\Delta F(I, J, P)] - 0.5 - K(I, J, P)\}, \quad (7)$$

$$\tau(I, J, P) = [N(I, J, P)+0.5]/2F(I, J, P) - [K(I, J, P)/2]\{[1/F(R, J, P)] - [1/F(I, J, P)]\}. \quad (8)$$

In the above expressions $K(I, J, P)$ may be written as

$$K(I, J, P) = IMP(J, P)/\rho(P)V(J, P) = IMP(J, P)\tau(J, P)/\rho(P_1)\lambda^2(P)L(J, P_1) \quad (9)$$

where $IMP(J, P)$ is the mechanical impedance of the transducer for the Jth velocity mode at pressure P.

It is evident from relation (8) that if the measurements are made near $F(R, J, P)$ any error in the estimation of $\tau(I, J, P)$ due to inaccurate knowledge of $K(I, J, P)$ becomes negligible.

By integrating relation (4) we obtain

$$\lambda(P) = \lambda(P_1)\exp[(P-P_1)/3B^T(P)]. \quad (10)$$

Two things should be noted regarding the derivation of (10) from (4): (i) In the definition of isothermal bulk modulus at a pressure P, one could obtain its value by either decreasing or increasing the pressure slightly; and (ii) when integrating (4) it must be remembered that it is implied in the definition of $B^T(P)$ that it remains constant over the range of integration P_1 to P. In expression (10) it is implied that the isothermal bulk modulus of a substance at pressure P has been obtained by decreasing the pressure from P to P_1. The expression for $\lambda(P)$ as derived above differs from that obtained by following either Cook's or Ruoff's procedures. The expression for $\lambda(P)$ that will be obtained by following Cook's or Ruoff's procedure may be given by

$$\lambda(P) = 1 + [\rho(1)L^2(1)]^{-1}\int_1^P [1+\Delta(P)] \times \{[4/\tau^2(3, P)] - [4/\tau^2(2, P)] - [1/\tau^2(1, P)]\}^{-1}dP, \quad (11)$$