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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

DATTATRAYA P. DANDEKAR

Washington State University, Pullman, Washington 99163

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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