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An Iterative Scheme to Estimate the Values of Elastic Constants of a Solid at High Pressures from the Sound Wave Velocity Measurements[1])

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The transit time measurements of sound wave velocities in a solid as a function of pressure contain all the possible information about the mechanical changes brought about in the solid due to the application of pressure. The present work gives a procedure to estimate accurately the values of the elastic constants of a solid from the transit time measurements as a function of pressure without *a priori* knowledge of the compressibility of the solid. When the transit time measurements are made as a function of pressure at more than two temperatures the procedure developed here also gives estimates for (i) the pressure derivative of the thermal expansion coefficient, (ii) the temperature derivative of the thermal expansion coefficient, and (iii) the pressure derivative of the specific heat, all as a function of pressure.

Messungen der Durchgangszeiten von Schallwellen in einem Festkörper als Funktion des Druckes enthalten alle möglichen Informationen über mechanische Veränderungen, die durch Anwendung von Druck im Festkörper bewirkt werden. Die vorliegende Arbeit gibt ein Verfahren an, um die Werte der elastischen Konstanten eines Festkörpers aus Messungen der Durchgangszeiten als Funktion des Druckes ohne a-priori-Kenntnisse der Kompressibilität genau abzuschätzen. Werden Messungen der Durchgangszeiten als Funktion des Druckes bei mehr als zwei Temperaturen durchgeführt, liefert das Verfahren außerdem: 1. die Druckableitung des thermischen Ausdehnungskoeffizienten, 2. die Temperaturableitung des thermischen Ausdehnungskoeffizienten, 3. die Druckableitung der spezifischen Wärme, alle als Funktion des Druckes.

1. Introduction

This paper presents an iterative procedure to estimate the values of the elastic constants of a crystalline solid at high pressures from the sound wave velocity measurements under the assumption that the concomitant compressibility measurements are either unavailable or unreliable. This procedure resembles the procedure developed by Cook [1] with regard to the use of the principle of self-consistent integration but differs with regard to the estimation of $\Delta(l, m, n, P, T)$ (cf. equation (7)). The iterative procedure presented here requires no restrictive assumptions when the sonic or ultrasonic measurements are made as a function of pressure at more than two temperatures. If, however, these measurements are made as a function of pressure at two temperatures, then we assume that the temperature derivatives of the linear thermal expansion coefficients are independent of pressure and they may be represented by their respective values at some lower pressure where they are known. Lastly, if the ultrasonic measurements are made as a function of pressure at only one tem-

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perature then an additional assumption must be made, i.e. the temperature derivatives of isothermal linear compressibilities are independent of pressure and they may be represented by their respective values at some lower pressure where they are known. For simplicity of presentation the analysis given in this paper refers to measurements of the transit-time of an elastic wave propagated in an anisotropic medium. No attempt is made to establish convergence of the procedure because it is generally difficult to do so for a numerical procedure unambiguousy since no explicit analytic expression can be obtained *a priori*. However, the iterative procedure presented in this paper predicts appropriate elastic constants whenever the data being analyzed are internally consistent; three examples discussed later confirm the utility of this procedure.

2. Conventions and Notations

For convenience, the elastic constants of a solid refer to the coordinate system (x, y, z) related to the crystal axes (a, b, c) as defined by the IRE Standards Committee [2]. The number of elastic constants (C_{ijkt}) necessary to characterize the elastic property of a solid depends upon the crystal class to which the solid belongs. The subscripts of these constants were contracted to (C_{pq}) by following the usual convention of writing the subscript $i\,j$, $k\,t = 11, 22, 33, 23, 12, 13$ by $p, q = 1, 2, 3, 4, 5, 6$ so as to represent these C_{pq} by a 6×6 matrix, denoted by $[C_{pq}]$. The corresponding 6×6 matrix of the elastic compliances S_{pq} may be obtained from C_{pq} by using the matrix relation between them, namely

$$[C_{pq}]\times[S_{pq}] = [I]\,, \tag{1}$$

where $[I]$ is a 6×6 unit matrix. The C_{pq}-matrices for the different crystal classes may be found in [3].

Notations

P	Pressure
T	Temperature
$\varrho(P, T)$	Density of a solid at pressure P and temperature T
$\chi(l, m, n, P, T)$	Linear compressibility of the solid in the direction whose direction cosines are given by l, m, and n at P and T
$\beta(l, m, n, P, T)$	Linear thermal expansion of the solid in the direction whose direction cosines are given by l, m, and n at P and T
$\chi(P, T)$	Volume compressibility of the solid at P and T
$\beta(P, T)$	Volume thermal expansion of the solid at P and T
$L(l, m, n, J, P, T)$	Width of the specimen used to measure the Jth velocity mode in the solid in the direction such that l, m, n determine the direction cosines at P and T
$\tau(l, m, n, J, P, T)$	Transit time of the Jth wave velocity mode corresponding to $L(l, m, n, J, P, T)$
$V(l, m, n, J, P, T)$	The Jth velocity in the solid in the direction whose direction cosines are l, m, and n at P and T
$\lambda(l, m, n, J, P, T)$	$= \dfrac{L(l, m, n, J, P_1, T)}{L(l, m, n, J, P, T)}$, where $P_1 < P$ and P equal to unity indicates one atmosphere pressure
$C_P(P, T)$	Specific heat of the solid at constant P and T.

The superscripts T and S attached to a quantity indicate its isothermal and adiabatic values, respectively.