First Pressure Derivatives of Polycrystalline Elastic Moduli: Their Relation to Single-Crystal Acoustic Data and Thermodynamic Relations

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This paper demonstrates that, for a given crystalline solid, the first pressure derivatives of polycrystalline elastic moduli can be predicted either from the corresponding derivatives of anisotropic single-crystal elastic constants or from their single-crystal third-order elastic constants. Theoretical relations for the isotropic polycrystalline acoustic data in terms of their single-crystal acoustic data are presented here for cubic, hexagonal, trigonal, and tetragonal crystals; these have been successfully applied for four cubic solids (Al, Cu, α-Fe, and MgO) and one hexagonal metal (Mg). It is shown for these solids that the calculated isotropic acoustic data agree essentially with experimental acoustic data determined on their polycrystalline specimens, thus establishing the validity of the theoretical relations. It is concluded that the acoustic data measured on *fully dense* polycrystalline specimens may be as useful as the single-crystal acoustic data in the study of the equation of state of solids, for example. And further, when anisotropic single-crystal acoustic data are available, these can be converted into isotropic polycrystalline acoustic data so that in their applications, the use of the acoustic data becomes more practical.

1. INTRODUCTION

The first pressure derivatives of the second-order elastic constants of a solid provide an important source of information for studies of lattice dynamics and of the general equation of state of the solid. However, measurements of these quantities are frequently limited by the unavailability of single-crystal specimens large enough for acoustic measurements to be made upon them. On the other hand, the fabrication of fully dense polycrystalline specimens has been possible in recent years for a number of materials, including metals, oxides, fluorides, sulfides (like β-ZnS), selenides (like ZnSe), and tellurides (like CdTe) as well as a large number of intermetallic compounds (like β-SiC and TiB_2). Acoustic measurements on polycrystalline specimens also are simpler in principle and of more practical use than those on single-crystal specimens, because the acoustic properties of polycrystals are *isotropic*, whereas those of single-crystals are *anisotropic*. Furthermore, for a polycrystalline specimen, measurements of only two sound velocities (one longitudinal and one transverse) as a function of hydrostatic pressure suffice to give the complete description of the second-order deformation behavior of the solid under hydrostatic pressure. The question then arises whether the acoustic data (e.g., the second-order elastic constants and their pressure derivatives) determined on polycrystalline specimens are equivalent to the corresponding quantities measured on single crystals. The primary purpose of this paper is to examine this question by computing, on the basis of a theoretical scheme,[1] polycrystalline

acoustic data from the corresponding single-crystal data, and comparing the result with experimentally determined values.

In the section immediately following, theoretical relations are presented for the first pressure derivatives of polycrystalline elastic moduli in terms of their single-crystal elastic constants and pressure derivatives for cubic, hexagonal, trigonal, and tetragonal crystals. Then, in Sec. 3, Sec. 2 is applied for four cubic solids and one hexagonal metal, since for these solids both the single-crystal and polycrystalline acoustic data are found in the literature. And, then in Sec. 4, the present work with cubic crystals is explicitly discussed for three thermodynamic boundary conditions (adiabatic, isothermal, and mixed). In Sec. 5, a procedure to calculate polycrystalline acoustic data from the single-crystal third-order elastic constants is presented for cubic crystals. And, finally in Sec. 6, the present work is discussed and its implications and possible applications in solid-state studies are indicated in brief.

2. RELATIONSHIP BETWEEN THE FIRST PRESSURE DERIVATIVES OF THE SINGLE-CRYSTAL ELASTIC CONSTANTS AND THOSE OF POLYCRYSTALLINE ELASTIC MODULI

The first pressure derivatives of polycrystalline elastic moduli in terms of the corresponding derivatives of the single-crystal elastic constants can be given as:

For the bulk modulus K,

$$dK^*/dp = \tfrac{1}{2}(dK_V/dp + dK_R/dp), \qquad (1)$$

and for the shear modulus G,

$$dG^*/dp = \tfrac{1}{2}(dG_V/dp + dG_R/dp). \qquad (2)$$

where

$$dK_V/dp = f_1(dc_{\mu\nu}/dp) \qquad (3a)$$

and

$$dK_R/dp = f_2(dc_{\mu\nu}/dp), \qquad (3b)$$

[1] (a) D. H. Chung, Proc. 4th Technical Society of Engineering Science, paper No. 5 (1966); (b) R. Hill, Proc. Phys. Soc. (London) **65**, 349 (1952). It is noted that Ref. 1a discusses the validity of the Voigt–Reuss–Hill approximation and its relation to other theoretical schemes of averaging the single-crystal elastic constants for a polycrystalline behavior. Other theoretical schemes referred here include a self-consistent method of Kröner (1958) and a variational method due to Hashin and Shtrikman (1962).