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Elastic Constants of and Wave Propagation in Antimony and Bismuth

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Ultrasonic wave velocities for 14 different modes were obtained on two differently oriented single-crystal antimony cubes from the time between successive unrectified radio-frequency pulse echoes. This redundant set of data was fitted by a least-squares technique to Voigt theory to yield the six room-temperature adiabatic elastic-stiffness constants. In units of 10^{10} dyn/cm^2, $c_{11}=99.4(1)$, $c_{33}=44.5(9)$, $c_{44}=39.5(5)$, $c_{66}=34.2(3)$, $c_{13}=26.4(4)$, and $c_{14}=+21.6(4)$, the positive sign for c_{14} following from our choice of positive Cartesian axes. When similarly treated, Eckstein, Lawson, and Reneker's bismuth data yield in these same units: $c_{11}=63.22$, $c_{33}=38.11$, $c_{44}=11.30$, $c_{66}=19.40$, $c_{13}=24.40\pm0.09$, $c_{14}=+7.20$. Also included are a visual method of fixing the laboratory coordinate system in antimony by means of an imperfect cleavage plane, a calculation of the pure-mode directions in the mirror plane, a simple formula for choosing the nonextraneous value of c_{13} for trigonal crystals having six independent elastic constants without resorting to lattice-stability criteria, and a calculation of the deviation of elastic-wave particle displacement and energy-flux directions from the propagation direction. For waves propagating in the (0,1,1) and (0,$\bar{1}$,1) directions, the particle-displacement deviations for antimony and bismuth do not exceed 15° and 13°, respectively, and corresponding energy-flux deviations up to 45° and 27° are obtained.

I. INTRODUCTION

In the well-designed experiment of Eckstein, Lawson, and Reneker[1] (hereinafter referred to as ELR), trigonal bismuth's six adiabatic elastic stiffness constants were determined from measurements of acoustic-wave propagation. An extension of their work to antimony seemed natural, and a recently determined set of antimony constants is desirable, considering both (1) the fact that currently available antimony crystals are purer and less strained than those available to Bridgman[2] and (2) the different measuring technique. The design of our experiment is essentially that of ELR, but our data are principally taken on just two differently oriented specimens, and our method of calculating the elastic constants differs in that we use a least-squares procedure. (For completeness and clarity of presentation we incorporate the basic data and equations given by ELR, and other material as appropriate; the reader is nevertheless referred to ELR for points not covered, and for additional references.) In addition, an inspection method of establishing laboratory axes in antimony is described; a simple formula is given for obtaining the nonextraneous value of c_{13}; the directions of pure-mode propagation in the mirror plane are evaluated; and the directions of particle displacement and energy flux for certain modes are calculated and compared with the wave-propagation direction. ELR's 14 bismuth velocities are also reanalyzed by our procedures, and a comparison between the two similar elements is made.

In the next section of this paper, some well-known crystallographic and cleavage data for antimony are introduced to provide a background for presenting the convention used for choosing coordinate axes in the crystal. This is followed by sections on the design of the experiment, experimental detail and the method of calculation of the constants. In the remaining sections the limitations of our analysis, the elastic constants, and acoustoelastic wave-propagation properties in anisotropic antimony and bismuth are discussed.

II. CRYSTALLOGRAPHIC DATA AND CLEAVAGE PROPERTIES OF ANTIMONY

Like bismuth, antimony's primitive cell is a 2 atom/cell rhombohedron (Fig. 1) with one atom at each corner and a ninth slightly displaced from the midpoint in the (1,1,1) direction. The nearest-neighbor distances[3] are 2.87 and 3.37 Å, the density is 6.7 g/cm^3, the rhombohedral angle is 57°6′, and the cell edge is 4.49 Å at room temperature.[4] It is brittle. The principal cleavage plane at room temperature is the (111) plane and fracture occurs between atoms having the larger nearest-neighbor distance; the secondary cleavage plane is of the (211) type indexed in the primitive cell,[5,6] and is relatively imperfect. These latter planes, spoken of as dominant secondary cleavage planes by one of us,[7] intersect the (111) plane in lines giving the directions of the three equivalent twofold axes. These axes are normal to the mirror planes which contain the trigonal and bisectrix axes. The plane's position in relation to a right-handed Cartesian coordinate system fixed in the crystal, or what is equivalent, the position of the plane's Laue spot reflection, can be used (see Sec. IV) to distinguish between two possible choices for such coordinate systems in which the signs of c_{14} and certain magnetoresistance coefficients[7] change. Our choice of coordinate system and the convention used to choose it

[1] Y. Eckstein, A. W. Lawson, and D. H. Reneker, J. Appl. Phys. **31**, 1535 (1960).

[2] P. W. Bridgman, Proc. Am. Acad. Arts Sci. **60**, 365 (1925).

[3] W. L. Bragg, *Atomic Structure of Minerals* (Cornell University Press, Ithaca, New York, 1937).

[4] C. S. Barret, P. Cucka, and K. Haefner, Acta Cryst. **16**, 451 (1963).

[5] C. Palache, H. Berman, and C. Frondel, *Dana's System of Mineralogy* (John Wiley & Sons, Inc., New York, 1955), Vol. 1.

[6] Relative to a hexagonal cell, this plane is of the (10$\bar{1}$4) type. Referred to a larger eight-atom-containing nearly face-centered cubic cell, it is of the (0$\bar{1}$1) type (also shown in Fig. 1).

[7] Seymour Epstein, J. Electrochem. Soc. **109**, 738 (1962); Seymour Epstein and H. J. Juretschke, Phys. Rev. **129**, 1148 (1963).