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Least-Squares Determination of the Elastic Constants of Antimony and Bismuth

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A least-squares determination of the elastic stiffness constants of antimony (using the data of Epstein and de Bretteville) and bismuth (using the data of Eckstein, Lawson, and Reneker) at room temperature was made by one of us (ERC). In the previous determination of the elastic constants of antimony and bismuth certain errors were not considered. They are considered in this paper. The antimony constants are: $c_{11}=101.3\pm1.6$; $c_{13}=29.2\pm2.2$; $c_{33}=45.0\pm1.5$; $c_{44}=39.3\pm0.7$; $c_{14}=20.9\pm0.4$; $c_{66}=33.4\pm0.6$; and $c_{12}=34.5\pm2.0$ all in units of 10^{10} dyn cm^{-2}. The bismuth constants in the same units are: $c_{11}=63.7\pm0.2$; $c_{13}=24.7\pm0.2$; $c_{33}=38.2\pm0.2$; $c_{44}=11.23\pm0.04$; $c_{66}=19.41\pm0.06$; $c_{12}=24.9\pm0.2$; $c_{14}=7.17\pm0.04$.

INTRODUCTION

The earlier paper of Epstein and de Bretteville on ultrasonic velocity measurements in antimony and bismuth at room temperature did not include a least-squares determination, in depth, of the elastic constants of these crystals.[1] Since the number of wave velocities measured for different propagation and polarization directions was larger than the number of elastic moduli for these crystals, such a determination would increase the accuracy of the computed values of the elastic constants. The least-squares determination is presented in this paper along with an analysis of the sources of experimental error and the final best values of the elastic constants of antimony and bismuth. The data for bismuth were taken from Eckstein, Lawson, and Reneker.[2]

VELOCITY ERRORS AND CORRECTIONS

The errors in measuring the echo time using the rf pulse-echo technique, in regard to the antimony measurement, are: (1) the uncertainty of measuring from the crest of one wave in one echo train (11 periods for shear and 20 periods for longitudinal waves) to the crest of the corresponding cycle in an adjacent train;

[1] S. Epstein and A. de Bretteville, Jr., Phys. Rev. **138**, A771 (1965).

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

(2) the transit time or round-trip time in the quartz transducer which is also intertwined with the phase shift caused by the reflection of the ultrasonic waves at the transducer including the bonding agent[3]; (3) the instrument error of the oscilloscope; (4) the error due to room-temperature changes on the transducer sample system; (5) misorientation of the crystal; (6) diffraction.

Item (1) above is the largest error of all and is assumed to be one cycle per round-trip time. The latter assumption is acknowledged to be both arbitrary and generous. The uncertainty of the velocity because of this is $|\Delta v_i^{\text{set}}| = |v_{i,m}^2/2l_if_r|$, where $v_{i,m}$ is the measured velocity without any correction, l_i the length of the sample, f_r is the resonant frequency or reciprocal of the period of the quartz transducer, and i refers to one of fourteen velocity measurements. If the error were assumed to be n integer cycles, the above formula would be multiplied by a factor n. The total error is the root-square sum of the measured error $\Delta v_{i,m}$ (due to the scattering of the measurements) and the $\Delta|v_i^{\text{set}}|$ described or $\Delta v_i = \{\Delta v_{i,m}^2 + (v_{i,m}^2/2f_rl_i)^2\}^{1/2}$. This formula is used to compute the total error in the measured velocity for antimony listed in Table I under measured velocity, plus a small misorientation correction given later in Table IV.

Eros and Reitz[4] have shown by a graphical analysis of the reflection and transmission of the rf pulse at the sample transducer interface, how to eliminate the error Δv_i^{set}, which they call the "transit time." Since the correction was not made in the antimony experiment[1] the correction formula Δv_i was necessary.

TABLE I. Observed velocities of sound in antimony at room temperature.

Symbol	Direction propagation	Mode	Measured velocity 10^5 cm/sec	Adjusted velocity 10^5 cm/sec
v_1[a]	x axis	Longitudinal	3.92 ± 0.08	3.891 ± 0.03
v_2[b,a]	x axis	Fast shear polarized along z	2.92 ± 0.14	2.930 ± 0.020
v_3[b,a]	x axis	Shear polarized along y	1.53 ± 0.04	1.508 ± 0.013
v_4	y axis	Longitudinal	3.99 ± 0.09	4.011 ± 0.026
v_5	y axis	Shear polarized along x	2.24 ± 0.05	2.23 ± 0.026
v_6	y axis	Shear polarized along z	2.24 ± 0.06	2.217 ± 0.018
v_7	z axis	Longitudinal	2.61 ± 0.09	2.591 ± 0.042
v_8	z axis	Degenerate shear	2.45 ± 0.08	2.423 ± 0.022
v_9	$\theta=45°\ \varphi=90°$	Longitudinal	3.19 ± 0.18	3.230 ± 0.032
v_{10}[b]	$\theta=45°\ \varphi=90°$	Shear polarized along x	2.92 ± 0.06	2.924 ± 0.020
v_{11}	$\theta=45°\ \varphi=90°$	Shear polarized along $\theta=45°$	1.28 ± 0.05	1.801 ± 0.040
v_{12}	$\theta=135°\ \varphi=-90°$	Longitudinal	4.14 ± 0.10	4.192 ± 0.025
v_{13}[b]	$\theta=135°\ \varphi=-90°$	Shear polarized along x	1.49 ± 0.04	1.518 ± 0.013
v_{14}	$\theta=135°\ \varphi=-90°$	Shear polarized along $\theta=135°$	1.51 ± 0.09	1.531 ± 0.041

[a] Dr. H. J. McSkimin kindly measured the three velocities, on this crystal by now accidentally severely damaged, by the buffered-pulse-superposition method. He obtained: $v_1=3.84(3)$; $v_2=2.93(0)$; and $v_3=1.47(4)$ all multiplied by 10^5 cm/sec. Only v_3 is outside the range of our experimental error.

[b] Although the inequality relations, $v_2 > v_{10}$ and $v_{13} > v_3$ are not satisfied for the measured velocity they are satisfied for the adjusted velocity, which are the more accurate values, obtained from the computer program. When the errors of the measured velocity are taken into account they are not incompatible with the inequality relations.

The transducer transit-time correction, item (2) above, was not made because of the uncertainty in the round-trip echo time mentioned in item (1). One can easily show that the transit-time error (neglecting bonding agent) is $-(f_r)^{-1}$, or one period, the minus sign meaning it should be subtracted from the round-trip echo time. The additional phase shift due to the transducer and bonding agent is probably small since the wave frequency is very close to the resonance frequency of the transducer, and the waves are assumed to be in a steady-state condition in the transducer. In order to check the latter assumption, the rf pulse width was increased from 2-μsec width at 5 MHz (10 periods) to about 3-μsec (15 periods), and finally to 4-μsec width (20 periods). In each case, the change if any in the first echo train was observed, as well as the echo time to the adjacent train. The results show that the shape of the first echo (other than a corresponding increase in the length of the echo train) appeared unaffected, in the first two cases, as well as the echo time, while this was not true for the last case.

The instrument error of the Tektronix 585A oscilloscope is given as: "Accuracy is typically within 1%, and in all cases within 3% of panel reading." The timing circuit of the oscilloscope was checked with a Tektronix Time Mark Generator 180-S1 and found to be well within 1%.

The effect of thermal expansion on the velocity in an antimony crystal, for a 20°C rise above room temperature, is negligible for the trigonal axis (maximum coefficient of expansion direction) and amounts to less than 0.1%.

The velocity error correction due to misorientation, which does not change the elastic constants over 1%, is given in Appendix A. The correct procedure would have been to determine the exact misorientation by x-ray back-reflection photographs and apply the correction to the velocity v_i instead of treating the correction as a random error as described in Appendix A. The χ^2 value, or $\sum(v_{i,\text{calc}} - v_{i,\text{obs}}/\Delta v_i)^2$, where $v_{i,\text{obs}}$ is the measured velocity with correction for misorientation, $v_{i,\text{calc}}$ is the calculated velocity obtained from Eq. (A1), and Δv_i is the error in velocity as described in detail above, decreased 34% (1.41 to 0.93) for bismuth after making the misorientation correction. One might expect only a small decrease in χ^2 because of the increase of Δv_i, but not such a large percentage change. In reality this is a gross simplification. Our basic assumption is that the χ^2 sum above should be a minimum, in order to obtain the best values of the six elastic constants. The consequence of this assumption, without going into detail, is that the coefficients of the six normal equations[5] used for determining the best value of the elastic constants contain the fourteen Δv_i as weights. Each

[3] H. J. McSkimin, J. Acoust. Soc. Am. **33**, 1 (1961).

[4] S. Eros and J. R. Reitz, J. Appl. Phys. **29**, 683 (1958).

[5] E. R. Cohen, K. M. Crowe, and J. W. M. DuMond, *Fundamental Constants of Physics* (Interscience Publishers, Inc., New York, 1957), pp. 235–244.

time Δv_i is changed, the elastic constants are completely redetermined, and this causes a corresponding change in the adjusted values $v_{i,\mathrm{calc}}$. The errors of the six elastic constants Δc_{ij} were reduced by the misorientation correction for bismuth.

In the case of antimony χ^2 became slightly worse by 7% (1.58 to 1.71) and the errors of the elastic stiffness constants for c_{11}, c_{13}, and c_{33} increased slightly, while those for c_{14}, c_{44}, and c_{66} decreased slightly. The trace relations for both semimetals were improved slightly by the application of this correction.

Papadakis has calculated curves for correcting v_7 for diffraction.[6] His graph is plotted in terms of the phase shift between echoes as a function of $S=z\lambda/a^2$, where z = path length in sample, λ = wavelength, and a = piston (transducer) radius for Waterman's anisotropy parameter b (the coefficient of $\theta^2 v_7$ in Appendix A). The calculation was not poslible as our b value for antimony is -9.8, which exceeds Papadakis's maximum value of -5. However, assuming the latter anisotropy parameter, the velocity correction for v_7 amounts to -0.1%.

CALCULATIONS AND RESULTS

The fourteen equations of Eckstein, Lawson, and Reneker (ELR)[2] were used by one of us (ERC) to determine the six elastic constants, by the method of least squares.[5] A preliminary calculation indicated that the measured velocity v_{11} (see Table I) was inconsistent, a conclusion which was apparent from the trace relations. It was therefore omitted and the remaining thirteen velocities were used to compute a "best" set of elastic constants: $c_{11}=101.3\pm1.6$; $c_{13}=29.2\pm2.2$; $c_{33}=45.0\pm1.5$; $c_{44}=39.3\pm0.7$; $c_{14}=20.9\pm0.4$; $c_{66}=33.4\pm0.6$; and $c_{12}=34.5\pm2.0$ all in units of 10^{10} dyn cm^{-2}. The isothermal correction is negligible. The importance of using a least-squares adjustment of the data in order to determine the elastic constants is that the adjusted velocities which may then be evaluated will satisfy *exactly* all the trace relations in theory.

The trace for the principal-axis-cut crystal of antimony is $T_{xy}=(26.00\pm0.24)\times10^{10}$ cm^2/sec^2 using the adjusted values from Table I, and the diagonal trace for the 45°-cut crystal is $T_{45°}=(22.22\pm0.19)\times10^{10}$ cm^2/sec^2.

Table I gives the values of the fourteen measured velocities and their least-squares adjusted values. The errors assigned to the adjusted velocities are computed from the full error matrix of the least-squares adjustment and should be used with care since the data are inter-related and cannot be treated as statistically independent. The elastic stiffness constant c_{13} as a result of this computation is found to be 10% higher than the previous finding.[1]

The compliances are $s_{11}=16.31$; $s_{33}=30.96$; $s_{44}=38.14$; $s_{12}=-6.15$; $s_{66}=44.93$; $s_{13}=-6.60$; and $s_{14}=-11.95$ all in units of 10^{-13} cm^2/dyn, and are in fair agreement with the data of Bridgman[7] who obtains $s_{11}=17.7$; $s_{33}=33.8$; $s_{44}=41$; $s_{12}=-3.8$; $s_{66}=43$; $s_{13}=-8.5$; and $s_{14}=-8.0$, all in units of 10^{-13} cm^2/dyn.

The fourteen equations were used with the same least-squares procedure as above to determine the six elastic constants of bismuth. The data of Eckstein, Lawson, and Reneker determined by the pulse-echo technique were used.[2] They state their velocities are accurate to better than 1%, and their principal error arises from the transducer transit-time correction. The "best" set of elastic constants is $c_{11}=63.7\pm0.2$; $c_{13}=24.7\pm0.2$; $c_{33}=38.2\pm0.2$; $c_{44}=11.23\pm0.04$; $c_{14}=7.17\pm0.04$; $c_{66}=19.41\pm0.06$; $c_{12}=24.9\pm0.2$, all in units of 10^{10} dyn/cm^2.

The compliances are $s_{11}=25.7$; $s_{33}=40.83$; $s_{44}=116.4$; $s_{12}=-8.13$; $s_{66}=67.6$; $s_{14}=-21.6$; $s_{13}=-11.33$, all in units of 10^{-13} cm^2/dyn. Bridgman's[8] results are $s_{11}=26.9$; $s_{33}=28.7$; $s_{44}=104.8$; $s_{12}=-14.0$; $s_{66}=81.2$; $s_{14}=16.0$; $s_{13}=-6.2$, all in units of 10^{-13} cm^2/dyn.

The principal-axis trace relation, or T_{xy} gives $(9.623\pm0.041)\times10^{10}$ cm^2/sec^2 from our least-squares results, versus $T_x=9.580$ and $T_y=9.654\times10^{10}$ cm^2/sec

TABLE II. Elastic-stiffness constants c_{ij} (10^{10} dyn/cm^2) of antimony at room temperature.

c_{11}	c_{13}	c_{14}	c_{33}	c_{44}	c_{66}	χ^2	Remarks
99.4(1)	26.4(4)	21.6(4)	44.5(9)	39.5(5)	34.2(5)	6.4	Near least squares.[a] No correction to experimental data.[b]
99.5±2.2	25.3±2.6	21.5±0.6	45.0±0.9	40.3±0.7	33.9±0.7	4.9	Least squares (ERC). No correction to experimental data.[b]
101.4±1.5	29.4±2.1	20.9±0.5	45.0±1.4	39.2±0.8	33.4±0.8	1.58	Least squares (ERC). Data corrected for "transit time."[c,d]
101.3±1.6	29.2±2.2	20.9±0.4	45.0±1.5	39.3±0.7	33.4±0.6	1.71[e]	Same as preceding plus an added misorientation correction.[f]

[a] Described in Ref. 1.
[b] Made by the rf pulse-echo technique (longitudinal principally at 10 MHz; shear principally at 5 MHz) of Ref. 1.
[c] Arbitrarily assumed to be ±1 cycle of pulse. See Ref. 4.
[d] The basic experimental data for this paper is slightly different from that chosen in Ref. 1.
[e] Data chosen as best in this paper.
[f] Equations (A5)–(A10).

[6] Emmanuel P. Papadakis (private communication).
[7] P. W. Bridgman, Proc. Am. Acad. Arts Sci. **60**, 363 (1925).
[8] Reference 7, p. 305.

TABLE III. Elastic constants c_{ij}(10^{10} dyn/cm^2) of bismuth at room temperature (experimental measurements of ELR used[a]).

c_{11}	c_{13}	c_{14}	c_{33}	c_{44}	c_{66}	χ^2	Remarks
63.50	24.50	7.23	38.10	11.30	19.40	1.7	No least squares. Transducer transit-time correction.[a]
63.22	24.40	7.20	38.11	11.30	19.40	2.6	Near least squares.[b] Transducer transit-time correction.[a]
63.7±0.3	24.6±0.2	7.20±0.04	38.1±0.2	11.26±0.04	19.38±0.07	1.4	Near least squares (ERC), plus preceding correction.
63.7±0.2	24.7±0.2	7.17±0.04	38.2±0.2	11.23±0.04	19.41±0.06	0.93[c]	Same as preceding plus misorientation correction.[d]

[a] See Ref. 2. Ultrasonic video pulse-echo technique used at 12 MHz.
[b] Described in Ref. 1.
[c] Data chosen as best in this paper.
[d] Equations (A5)–(A10).

for Eckstein, Lawson, and Reneker.[2] The 45°-cut crystal trace relation gives $T_{45°}=(7.911\pm0.022)\times10^{10}$ cm^2/sec^2 from least squares, while ELR obtain $T_{45°}=7.974$ for $\varphi=90°$, and $T_{135°}=7.899\times10^{10}$ cm^2/sec^2 for $\varphi=-90°$.

Tables II and III summarize the effects of different data processing on the elastic-stiffness constants of antimony and bismuth, respectively, and represent additional measurements on the original specimens taken by one of us (deB).

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APPENDIX A: MISORIENTATION CORRECTION

The velocity error due to misorientation can be calculated from the following determinant for point group $\bar{3}m$, where $x=\rho v^2$, ρ is the density, and v the sonic velocity.[9]

$$\begin{vmatrix} A-x & H & G \\ H & B-x & F \\ G & F & C-x \end{vmatrix}=0\,. \quad \text{(A1)}$$

Here,

$$A=c_{11}\sin^2\theta\cos^2\varphi+\tfrac{1}{2}(c_{11}-c_{12})\sin^2\theta\sin^2\varphi +c_{44}\cos^2\theta+2c_{14}\sin\theta\cos\theta\sin\varphi\,,$$

$$B=\tfrac{1}{2}(c_{11}-c_{12})\sin^2\theta\cos^2\varphi+c_{11}\sin^2\theta\sin^2\varphi +c_{44}\cos^2\theta-2c_{14}\sin\theta\cos\theta\sin\varphi\,,$$

$$C=c_{44}\sin^2\theta+c_{33}\cos^2\theta\,,$$

$$F=c_{14}\sin^2\theta(1-2\sin^2\varphi)+(c_{13}+c_{44})\sin\theta\cos\theta\sin\varphi\,,$$

$$G=2c_{14}\sin^2\theta\sin\varphi\cos\varphi+(c_{13}+c_{44})\sin\theta\cos\theta\cos\varphi\,,$$

and

$$H=\tfrac{1}{2}(c_{11}+c_{12})\sin^2\theta\sin\varphi\cos\varphi+2c_{14}\sin\theta\cos\theta\cos\varphi\,.$$

θ is the angle between a direction of propagation and the positive z axis, φ is the angle in the basal plane measured from the positive x axis counterclockwise to the projection of the direction of propagation on the basal plane.

The equations for the three velocities are, neglecting G and H which are small and would be zero for a perfectly oriented principal axis and 45°-cut crystal,

$$\rho v^2=A\,, \quad \text{(A2)}$$

$$\rho v^2=(B+C)+\{(B-C)^2+4F^2\}^{1/2}\,, \quad \text{(A3)}$$

$$\rho v^2=(B+C)-\{(B-C)^2+4F^2\}^{1/2}\,. \quad \text{(A4)}$$

Equations (A2)–(A4) were differentiated with respect to velocity in terms of θ and φ, and solved for the error $\pm\Delta v_i$ by inserting the appropriate elastic-stiffness constants c_{ij}, velocities v_i, and the value $\Delta\theta=\pm1°$ for

TABLE IV. Velocity errors due to misorientation for antimony and bismuth.

Symbol	Antimony 10^5 cm/sec	Bismuth 10^5 cm/sec
$\pm\Delta v_1$	0.00	0.000
$\pm\Delta v_2$	0.00	0.000
$\pm\Delta v_3$	0.00	0.000
$\pm\Delta v_4$	0.00	0.000
$\pm\Delta v_5$	0.00	0.000
$\pm\Delta v_6$	0.00	0.000
$\pm\Delta v_7$	0.00	0.000
$\pm\Delta v_8$	0.02	0.012
$\pm\Delta v_9$	0.01	0.006
$\pm\Delta v_{10}$	0.00	0.005
$\pm\Delta v_{11}$	0.03	0.010
$\pm\Delta v_{12}$	0.01	0.008
$\pm\Delta v_{13}$	0.01	0.008
$\pm\Delta v_{14}$	0.03	0.002

[9] J. B. Wachtman, Jr., W. E. Tefft, D. G. Lam, Jr., and R. P. Stinchfield, J. Res. Natl. Bur. Std. **64A**, 219 (1960).

antimony and bismuth. The results are tabulated in Table IV.

The velocity error for v_8 was calculated from Waterman's formula $\Delta v_8 = v_8\theta c_{14}/c_{44}$, after putting $c_{25}=0$, where θ is the polar misorientation angle, or $\Delta\theta$ in our notation.[10] The value for Δv_8 of antimony and bismuth was inserted in Table IV. Waterman's expression for the increase in the longitudinal velocity along the trigonal axis is $\Delta v_7 = v_7\theta^2(2c_{44}+c_{13}-c_{33})/2c_{33}(c_{33}-c_{44})$. The value for antimony is $\Delta v_7 = 0.01\times 10^5$ cm/sec, and the corresponding value for bismuth 0.002×10^5 cm/sec, were added to their respective values of v_7 and inserted in Table I. Waterman's expression for Δv_7 is a systematic term and amounts to about $\frac{1}{4}\%$ of v_7 for antimony and $\frac{1}{10}\%$ for bismuth. Apparently Δv_7 cannot explain the 34% drop in χ^2 when the misorientation correction is applied to bismuth, because it is so small. The change comes about primarily for bismuth, as mentioned in the text, because of the influence of the weighting factors on the "best" values for the elastic-stiffness constants.

Equations (A5)–(A10) give the velocity errors for the 45°-cut crystal and are to first order in θ. The second-order terms in φ were neglected. There were no second-order terms in θ. The G and H terms in Eq. (A1) would add nothing to Eqs. (A5)–(A10) if they had been included. The reason is that they would occur as products and squares such as G^2, H^2, and $2GHF$, which on differentiation become $2GdG$, $2HdH$, $2HFdG$, and all equal zero because G and H contain $\cos\varphi$ ($\varphi=\pm 90°$ for propagation in the bisectrix) as a coefficient.

$$\Delta v_9 = \left\{(c_{11}-c_{33}) + \frac{2(\frac{1}{2}c_{11}-\frac{1}{2}c_{33}-c_{14})(c_{11}+c_{33}-2c_{44})-4(c_{13}+c_{44}-c_{14})c_{14}}{2\{(\frac{1}{2}c_{11}-\frac{1}{2}c_{33}-c_{14})^2+(c_{13}+c_{44}-c_{14})^2\}^{1/2}}\right\} d\theta/4\rho v_9, \tag{A5}$$

$$\Delta v_{10} = (c_{66}-c_{44})d\theta/2\rho v_{10}, \tag{A6}$$

$$\Delta v_{11} = \left\{(c_{11}-c_{33}) - \frac{2(\frac{1}{2}c_{11}-\frac{1}{2}c_{33}-c_{14})(c_{11}+c_{33}-2c_{44})-4(c_{13}+c_{44}-c_{14})c_{14}}{2\{(\frac{1}{2}c_{11}-\frac{1}{2}c_{33}-c_{14})^2+(c_{13}+c_{44}-c_{14})^2\}^{1/2}}\right\} d\theta/4\rho v_{11}, \tag{A7}$$

$$\Delta v_{12} = \left\{(c_{33}-c_{11}) + \frac{2(\frac{1}{2}c_{11}-\frac{1}{2}c_{33}+c_{14})(2c_{44}-c_{11}-c_{33})+4(c_{13}+c_{44}+c_{14})c_{14}}{2\{(\frac{1}{2}c_{11}-\frac{1}{2}c_{33}+c_{14})^2+(c_{13}+c_{44}+c_{14})^2\}^{1/2}}\right\} d\theta/4\rho v_{12}, \tag{A8}$$

$$\Delta v_{13} = (c_{44}-c_{66})d\theta/2\rho v_{13}, \tag{A9}$$

$$\Delta v_{14} = \left\{(c_{33}-c_{11}) - \frac{2(\frac{1}{2}c_{11}-\frac{1}{2}c_{33}+c_{14})(2c_{44}-c_{11}-c_{33})+4(c_{13}+c_{44}+c_{14})c_{14}}{2\{(\frac{1}{2}c_{11}-\frac{1}{2}c_{33}+c_{14})^2+(c_{13}+c_{44}+c_{14})^2\}^{1/2}}\right\} d\theta/4\rho v_{14}. \tag{A10}$$

The equations for the velocity error for the x and y axes contained second-order corrections, were small, and therefore were neglected.

The misorientation correction, shown in Table IV, was incorporated into the formula for Δv_i in the text, and improved the χ^2 value for bismuth from 1.409 to 0.929 while the corresponding values for antimony were worsened slightly from 1.582 to 1.708. The misorientation correction improved the equality of the trace relations for antimony and bismuth, and reduced the errors slightly for the elastic-stiffness constants of the latter, while for antimony, half were reduced and half increased slightly. The correction has at the maximum a 1% effect on the antimony elastic constants. For example, if they were not incorporated into the least-squares calculation, c_{13} would decrease by 0.2×10^{10} dyn/cm². Likewise for bismuth, c_{13} and c_{33} would decrease by 0.1×10^{10} dyn/cm².

[10] P. C. Waterman, Phys. Rev. **113**, 1247 (1959).