COMPRESSIBILITY OF HEXAGONAL AgI



hkl	$\beta_{hkl} \ 10^{-6}/\text{bar}$	$s_{ep} \ 10^{-4}$	$\pm \Delta \beta \ 10^{-6}/\text{bar}$	e 10 ⁻⁶ /bar	$\pm (\Delta \beta + e) \ 10^{-6}/\text{bar}$
002	1.258	3.9	0.18	0.17	0.35
105	1.126	3.5	0.16	0.01	0.17
103	1.050	3.7	0.17	0.15	0.32
203	1.217	2.9	0.13	0.10	0.23
112	1.344	2.8	0.13	0.02	0.15
213	1.312	3.0	0.14	0.05	0.19
211	1.560	2.8	0.13	0.12	0.25
110	1.495	5.4	0.25	0.04	0.29

TABLE 1. Experimental Linear Compressibilities and Error Analysis

6021

3200

DAVIS AND BLAIR



6022

Fig. 3. One quadrant of the linear compressibility surface for hexagonal AgI. See Table 1 for fitting uncertainty.

squares. This fit yields the compressibility constants $\beta_a = (1.46 \pm 0.42) \times 10^{-6}$ /bar and $\beta_o = (1.09 \pm 0.32) \times 10^{-6}$ /bar. There is some scatter to the plot, and the data actually fit a parabolic relationship much better. The rather large errors attendant to β_a and β_o result from both scatter about the original plots of $\Delta l/l_o$ versus P and the scatter about the quadric. Table 1 also includes the calculated standard error of estimate s_{ep} obtained from the linear regression analysis of the β_{hkl} values. If one considers the initial unaveraged data which resulted in the composite plots of Figure 2, the maximum value of s_{ep} obtained was 5.4×10^{-4} and was that for the 103 spacing.

Errors observed in scattering of the compression plots, however, are not valid measures of the uncertainties in β_{nk1} for each spacing. This is adequately given by *Dixon and Massey* [1957, p. 194].

$$\Delta \beta_{hkl} = \frac{t_{0.90} s_{ep}}{s_p (N-1)^{1/2}}$$

at the 90% confidence level of the assumed t distribution, with two degrees of freedom. The uncertainties $\Delta \beta_{hhl}$ for each spacing are given in Table 1.

Calculation of β_a and β_c by least-squares fit of the compressibility quadric (equation 1) to the β_{kkl} values of Table 1 results in a fitting error *e* given by

$$e = \beta_a(1 - l^2) + \beta_c l^2 - \beta_{hkl}'$$

hich is also additive to s_{ep} in terms of the

W

uncertainty in β_{hkl} calculated from the compressibility quadric.

Table 1 shows that the uncertainties stemming from the direct measurements lie between 8 and 17%, but those $(\Delta\beta_{kkl} + e)$ associated with β' calculated from the quadric parameters run as high as 30%. The source of the uncertainties is obviously experimental and lies in (1) slight variations in sample height and (2) random errors, including chart-reading limitations imposed by low Bragg-angle measurements.

The only published data for the elasticity of hexagonal AgI is a volume compressibility of 4.11×10^{-6} /bar given by Richards and Jones [1909] for iodyrite (naturally occurring hexagonal AgI). J. Wachtman, quoted in Burley [1964], gives a value of 10.1 \times 10⁻⁶/bar for polycrystalline material. No statement as to phase composition is given, but in view of the sample preparation it was most likely a mixture of cubic and hexagonal forms. The present linear compressibility data yield a volume compressibility of 4.01×10^{-6} /bar, which is in good agreement with the data of Richards and Jones. However, the poor agreement with Wachtman's value should be better, in view of the close similarity of structures of the two AgI polymorphs.

Acknowledgments. We acknowledge C. L. Tollinger's fine machine work in the construction of the apparatus. We also thank E. Hoskins for helpful suggestions and discussion.

This program was financially supported by the National Science Foundation (GP-5075) and the Bureau of Reclamation (14-06-D-5979).

References

- Burley, G., An X-ray determination of the Debye temperature of silver iodide, J. Phys. Chem. Solids, 25, 629, 1964.
- Davis, B. L., and D. N. Blair, Compressibility and elastic compliances of hexagonal silver iodide (abstract), Trans. Am. Geophys. Union, 41, 185, 1968.
- Davis, B. L., and M. J. Walawender, X-ray observation of chemical and polymorphic equilibria under hydrostatic pressures, J. Phys. Chem. Solids, in press, 1968.
- Dixon, W. J., and F. J. Massey, Jr., Introduction to Statistical Analysis, 488 pp., McGraw-Hill Book Company, New York, 1957.
- Richards, T. W., and G. Jones, The compressibilities of the chlorides, bromides, and iodides of sodium, potassium, silver, and thallium, J. Am. Chem. Soc., 31, 158, 1909.
- Slater, J. C., Compressibility of the alkali halides, *Phys. Rev.*, 23, 488, 1924.

(Received March 27, 1968; revised June 6, 1968.)