

Fig. 2. Linear strain  $\Delta l/l_0 = \Delta 2\theta/2\theta_0$  versus internal pressure for (A) 112, (B) 203, (C) 105, (D) 213, (E) 211, (F) 110 and 002, and (G) 103 diffraction spacings for hexagonal AgI. See Table 1 for uncertainties.

TABLE 1. Experimental Linear Compressibilities and Error Analysis

$hkl$	$\beta_{hkl} 10^{-6}/\text{bar}$	$s_{ep} 10^{-4}$	$\pm \Delta\beta 10^{-6}/\text{bar}$	$e 10^{-6}/\text{bar}$	$\pm(\Delta\beta + e) 10^{-6}/\text{bar}$
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

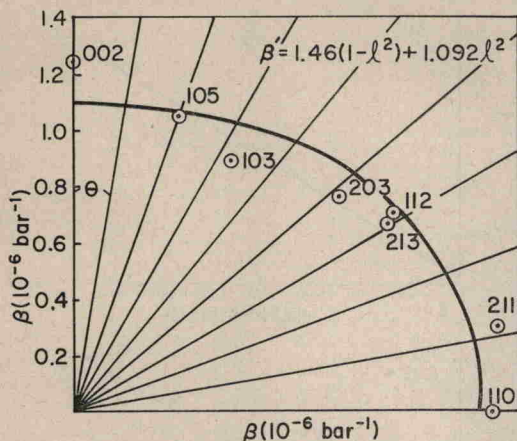


Fig. 3. One quadrant of the linear compressibility surface for hexagonal AgI. See Table 1 for fitting uncertainty.

squares. This fit yields the compressibility constants  $\beta_a = (1.46 \pm 0.42) \times 10^{-6}/\text{bar}$  and  $\beta_c = (1.09 \pm 0.32) \times 10^{-6}/\text{bar}$ . There is some scatter to the plot, and the data actually fit a parabolic relationship much better. The rather large errors attendant to  $\beta_a$  and  $\beta_c$  result from both scatter about the original plots of  $\Delta l/l_0$  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  $\beta_{hkl}$  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  $5.4 \times 10^{-4}$  and was that for the 103 spacing.

Errors observed in scattering of the compression plots, however, are not valid measures of the uncertainties in  $\beta_{hkl}$  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  $\Delta\beta_{hkl}$  for each spacing are given in Table 1.

Calculation of  $\beta_a$  and  $\beta_c$  by least-squares fit of the compressibility quadric (equation 1) to the  $\beta_{hkl}$  values of Table 1 results in a fitting error  $e$  given by

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

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

uncertainty in  $\beta_{hkl}'$  calculated from the compressibility quadric.

Table 1 shows that the uncertainties stemming from the direct measurements lie between 8 and 17%, but those  $(\Delta\beta_{hkl} + e)$  associated with  $\beta'$  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  $4.11 \times 10^{-6}/\text{bar}$  given by *Richards and Jones* [1909] for iodyrite (naturally occurring hexagonal AgI). *J. Wachtman*, quoted in *Burley* [1964], gives a value of  $10.1 \times 10^{-6}/\text{bar}$  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  $4.01 \times 10^{-6}/\text{bar}$ , 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.

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