ΦΥΣΙΚΗ.— **Internal Strain of Ge,** by *G. E. Zardas* and *C. N. Koumelis* *, διὰ τοῦ Ἀκαδημαϊκοῦ κ. Καίσαρος Ἀλεξοπούλου.

ABSTRACT

The problem of the Internal Strain is examined in Ge by measuring the displacement of an X-Ray beam diffracted on it under an uniaxial stress along the [111] direction. The law of the change of the bond lengths $b_{\langle 11\bar{1}\rangle}$ versus the applied stress was determined. The value of the bond bending constant ζ was found to be 0.88.

INTRODUCTION

The problem of the Internal Strain in crystals with tetrahedral bonds consists in achieving the strain $\varepsilon'_{[111]}$ of the tetrahedral bond for a given macroscopic strain $\varepsilon_{[111]}$ along this bond. The strain $\varepsilon'_{[111]}$ is generally not equal to the macroscopic strain $\varepsilon_{[111]}$, but is connected to it by: (1) (2) (3)

$$\varepsilon'_{[111]} = \varepsilon_{[111]} - \zeta \cdot \varepsilon_{[111]}$$

where: $0 \leqslant \zeta \leqslant 1$ is the so called bond bending constant.

The bond bending constant of Ge and Si was found with the help of X-Rays for the longitudinal and transverse case. (4) (5) The experiment was extended to the zinc-blende structure, specifically to Sbln (6) and GaAs. (7) (8).

This experiment, which is still in progress, examines the change of the bond $b_{[11\bar{1}]}$ under the stress $\vec{\tau}_{[111]}$. For reasons of symmetry, the same law holds for all bonds $b_{\langle 11\bar{1}\rangle}$.

CALCULATIONS

Under a sress $\vec{\tau}_{[111]}$, a cubic crystal becomes rhombohedral (Fig. 1). In Fig. 2 we present the atomic positions on the crystallographic plane $(1\,\bar{1}\,0)$ of the strained diamond structure crystal under the stress $\vec{\tau}_{[111]}$, assuming an internal strain.

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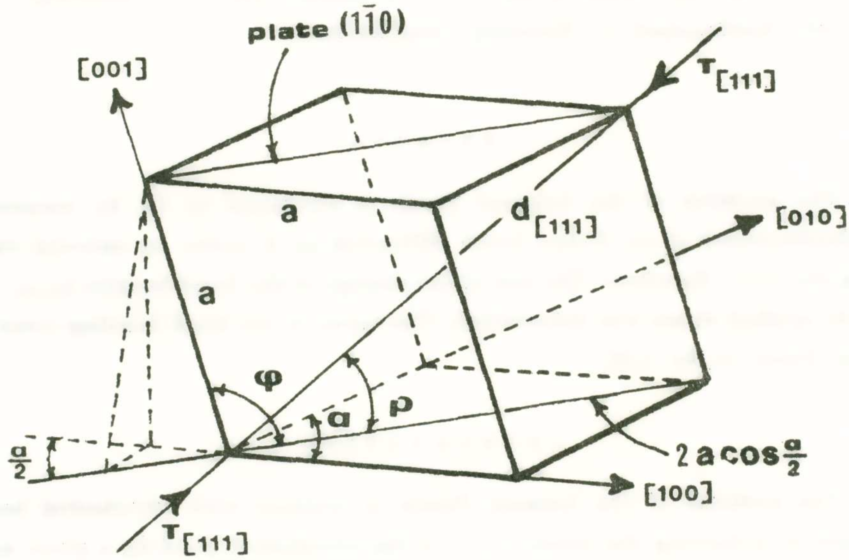

Fig. 1 Cubic crystal under the stress $\vec{\tau}_{[111]}$ becomes rhombohedral

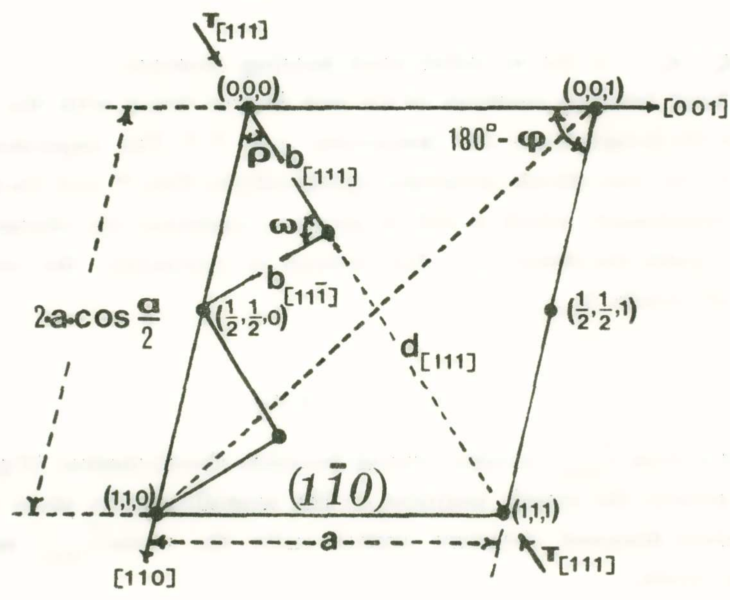

Fig. 2 The crystallographic plane (1 $\bar{1}$ 0) of the diamond under the stress $\vec{\tau}_{[111]}$ when $\zeta \neq 0$

From Fig. 1 we have

$$\cos\varphi = \frac{\cos\alpha}{\cos\frac{\alpha}{2}} \qquad (1\alpha)$$

$$d^2_{[111]} = 3 \cdot a^2 \cdot (1 + 2 \cdot \cos\alpha) \qquad (1\beta)$$

$$\cos\rho = \sqrt{\frac{2}{3} \cdot \frac{1 + 2 \cdot \cos\alpha}{1 + \cos\alpha}} \qquad (1\gamma)$$

Fig. 2 leads to:

$$b^2_{[11\bar{1}]} = \frac{a^2}{4} + \frac{a^2_0}{16} \cdot \left[1 + (1 + \zeta) \cdot \varepsilon_{[111]} \right] \cdot \left[(3 \cdot \zeta - 1) \cdot \varepsilon_{[111]} - 1 \right] \qquad (2)$$

where a_0 is the lattice constant of the unstrained crystal.

If the lattice constant a does not follow the strain tensor and is unknown function of the strain $\varepsilon_{[111]}$, equation (2) does not solve the problem, but a further experiment is neeeded for determination of the relation

$$a = a\,[\varepsilon_{[111]}]$$

EXPERIMENTAL PROCEDURE

On the photographic plate (Fig. 3) we measure the distance S of the reflection (hkl) versus the stress $\vec{\tau}_{[111]}$. The Bragg law gives for a rhombohedral crystal: (9)

$$\frac{2 \cdot a \cdot \sin\theta \cdot \sqrt{(1 - \cos\alpha) \cdot (1 + 2 \cdot \cos\alpha)}}{\sqrt{h^2 + k^2 + l^2 + [h^2 + k^2 + l^2 - 2 \cdot (h \cdot k + k \cdot l + l \cdot h)] \cdot \cos\alpha}} = \lambda$$

The last equation, the equation (1β) and the relation

$$d_{[111]} = a_0 \cdot \sqrt{3} \cdot [1 + \varepsilon_{[111]}]$$

lead to:

$$\cos\alpha = \frac{1 - \dfrac{h^2 + k^2 + l^2}{4 \cdot a_0^2 \cdot [1 + \varepsilon_{[111]}]^2 \cdot \sin^2\theta} \cdot \lambda^2}{1 + \dfrac{h^2 + k^2 + l^2 - 2 \cdot (h \cdot k + k \cdot l + l \cdot h)}{4 \cdot a_0^2 \cdot [1 + \varepsilon_{[111]}]^2 \cdot \sin^2\theta} \cdot \lambda^2}$$

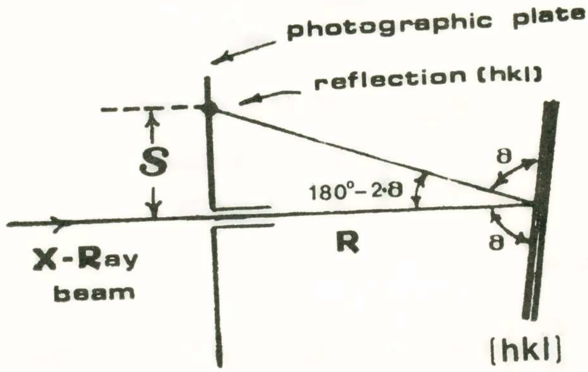

Fig. 3 The geometry of the reflection (hkl)

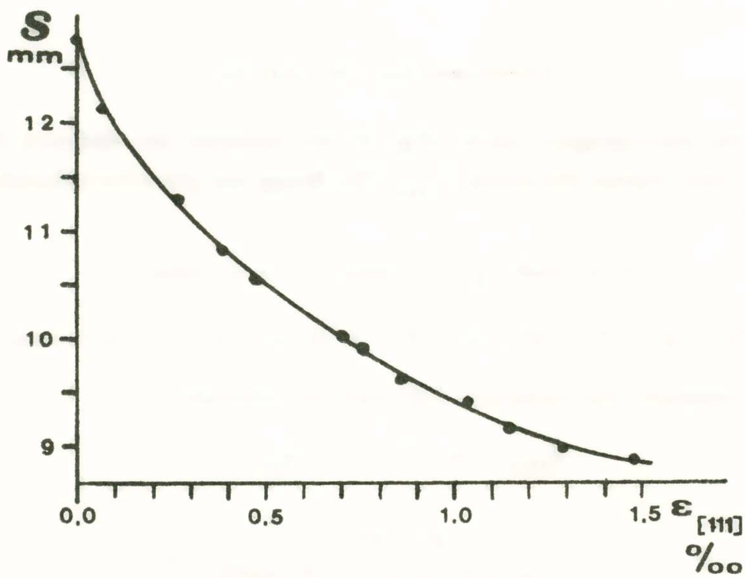

Fig. 4 The curve S=S $[\varepsilon_{[111]}]$ for the reflection (11 11 $\bar{3}$). (R = 150 mm)

$$a^2 = a_0^2 \cdot [1 + \varepsilon_{[111]}]^2 \cdot \frac{1 + \dfrac{h^2 + k^2 + l^2 - 2 \cdot (h \cdot k + k \cdot l + l \cdot h)}{4 \cdot a_0^2 \cdot [1 + \varepsilon_{[111]}]^2 \cdot \sin^2\theta} \cdot \lambda^2}{3 - \dfrac{(h + k + l)^2}{4 \cdot a_0^2 \cdot [1 + \varepsilon_{[111]}]^2 \cdot \sin^2\theta} \cdot \lambda^2}$$

The last equation gives the lattice constant a, versus θ and $\varepsilon_{[111]}$, which can be experimentally determined. The Bragg angle θ is determined from Fig. 3:

$$\theta = \frac{1}{2} \cdot \arctan\left(-\frac{S}{R}\right)$$

The strain $\varepsilon_{[111]}$ is determined from the relation: (10) (11) (12)

$$\varepsilon_{[111]} = \left[\frac{s_{11} + 2 \cdot s_{12}}{3} + \frac{s_{44}}{3}\right] \cdot \tau_{[111]}$$

RESULTS

We have experimented on Ge, the elastic constants of which are: (13)

$$s_{11} = 0.978 \cdot 10^{-12} \frac{cm^2}{dyne}$$

$$s_{12} = -0.266 \cdot 10^{-12} \frac{cm^2}{dyne}$$

$$s_{44} = 1.490 \cdot 10^{-12} \frac{cm^2}{dyne}$$

For Mo$k\alpha_2$ radiation, the reflection ($11\ 11\ \bar{3}$) was chosen because it gives the large value:

$$\tan\theta = 23.5320$$

Figure 4 shows the experimental curve of the distance S of the reflection ($11\ 11\ \bar{3}$) from the center of the photographic plate, versus the strain $\varepsilon_{[111]}$, for $R = 150$ mm.

Figure 5 shows the corresponding Bragg angle θ versus $\varepsilon_{[111]}$. From Fig. 5 we calculate the lattice constant a, shown in Fig. 6. The curve is not linear and moreover has a minimum around $\varepsilon_{[111]} = 0.8\ ^0/_{00}$. We cannot give an explanation for this behavior.

By trial and error the curve of Fig. 6 could be expressed by the equation:

$$a^2 + K \cdot a \cdot \varepsilon_{[111]} + L \cdot \varepsilon^2_{[111]} + M \cdot a + N \cdot \varepsilon_{[111]} + P = 0$$

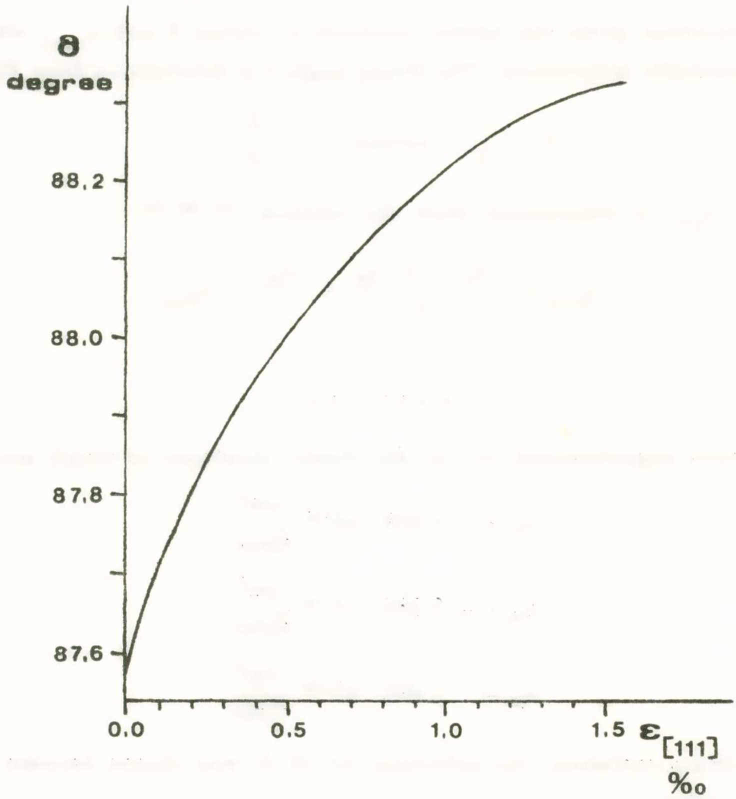

Fig. 5 The Bragg angle θ of the reflection (11 11 $\bar{3}$) under strain $\varepsilon_{[111]}$

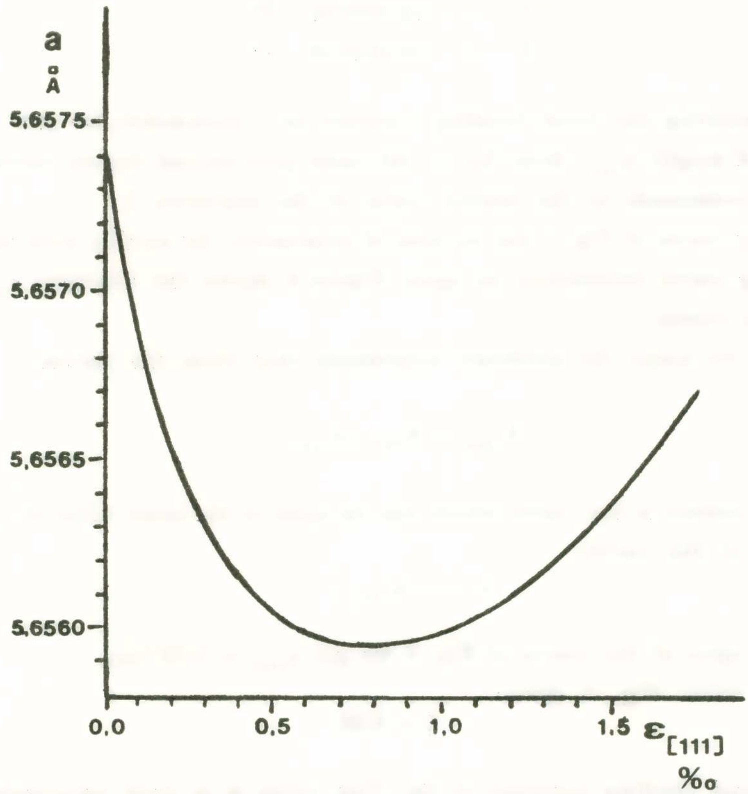

Fig. 6 The curve $a = a\,[\varepsilon_{[111]}]$

With an electronic calculator we obtain the follow values for the coefficients:

$$\begin{aligned} K &= 2.217299 \ \text{Å} \\ L &= 6.356274 \ \text{Å}^2 \\ M &= -11.316211 \ \text{Å} \\ N &= -12.530700 \ \text{Å}^2 \\ P &= 32.014158 \ \text{Å}^2 \end{aligned}$$

Considering the bond bending constant as a parameter, we plot in Fig. 7 the bond length $b_{[11\bar{1}]}$ from Eq. 2. All cases give second degree curves. One of them corresponds to the correct value of the unknown ζ.

Every curve of Fig. 7 has an axis of symmetry; its section with the corresponding curve determines an apex. Figure 8 shows the abscissas $\varepsilon_{[111]_x}$ of the apexes versus ζ.

Now we make the arbitrary hypothesis that from the curves

$$b_{[111]} = b_{[111]} \left[\varepsilon_{[111]}, \zeta\right]$$

of Fig. 7, correct is the curve which has its apex at the same value of $\varepsilon_{[111]_x}$ as the apex of the curve:

$$a = a \left[\varepsilon_{[111]}\right]$$

From the apex of the curve of Fig. 6 we get $\varepsilon_{[111]} = 0.69\ ^{0}/_{00}$.
For this value Fig. 8 gives:

$$\zeta = 0.88$$

for the bond bending constant of Ge. This value is in good agreement with those referred in the literature [4] [5] [14] and with the theoretically calculated one [15].

We note that in this experiment, the value of the bond bending constant was found without measuring the X - Ray intensity, but solely from the position of the Bragg reflection.

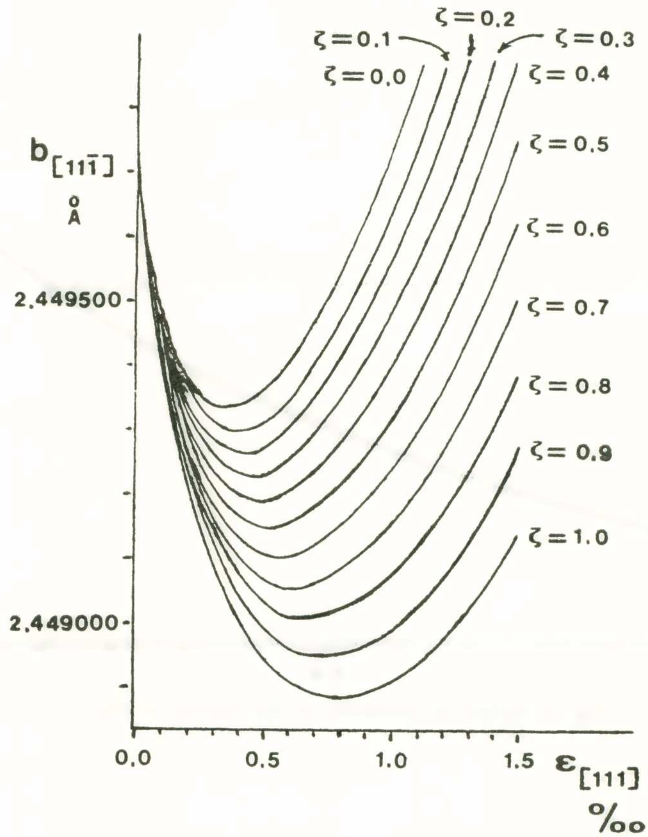

Fig. 7 The group of the curves $b_{[11\bar{1}]} = b_{[11\bar{1}]}\ [\varepsilon_{[111]}]$

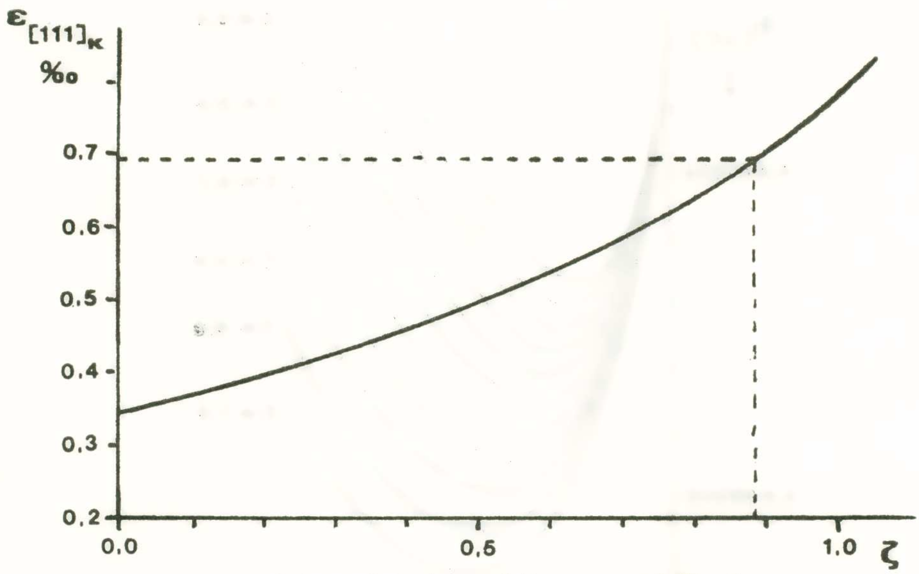

Fig. 8 Values of abscissas of the apexes of Fig. 7

ΠΕΡΙΛΗΨΙΣ

Η ΕΣΩΤΕΡΙΚΗ ΠΑΡΑΜΟΡΦΩΣΙΣ ΕΙΣ ΤΟ GE

Εἰς τὸ παρὸν πείραμα ἐξητάσθη τὸ πρόβλημα τῆς ἐσωτερικῆς παραμορφώσεως εἰς τὸ Ge διὰ μετρήσεως τῆς μετατοπίσεως γραμμῆς ἀκτίνων Roentgen λόγῳ ἐξασκήσεως μονοαξονικῆς τάσεως κατὰ τὴν διεύθυνσιν [111]. Εὑρέθη ὁ νόμος τῆς μεταβολῆς τῶν δεσμῶν $b_{\langle 11\bar{1}\rangle}$ συναρτήσει τῆς ἐφαρμοζομένης τάσεως, εὑρέθη δὲ ἡ τιμὴ 0.88 διὰ τὴν σταθερὰν κάμψεως δεσμῶν ζ.

REFERENCES

1. Max Born and K. Huang, "Dynamical Theory of Crystal Lattices" p. 134, Oxford, Clarendon Press, 1954.
2. L. Kleinman, Phys. Rev. 128, 2614, 1962.
3. L. Kleinman, Phys. Rev. 130, 2283, 1963.
4. A. Segmüller, Phys. Cond. Matter 3, 18, 1964.
5. A. Segmüller and H. R. Neyer, Phys. Kond. Matterie 4, 63, 1965.
6. C. N. Koumelis, Thesis, Athens, 1965.
7. C. N. Koumelis and E. K. Rozis, (a) Acta Cryst. A31, 84 (1975), (b) Acta Cryst. A32, 170, 1976.
8. C. N. Koumelis, G. E. Zardas, C. A. Londos and D. L. Leventouri, Acta Cryst. A32, 306, 1976.
9. B. D. Cullity, "Elements of X-Ray Diffraction" p. 459, Addison Wesley Publishing Co, 1967.
10. A. E. Love, "The Mathematical Theory of Elasticity" p. 80, Dover, 1944.
11. C. Kittel, "Introduction to Solid State Physics" p. 118, John Wiley, 1968.
12. H. Kolsky, "Stress Waves in Solids" p. 10, Dover Publications, 1963.
13. H. B. Huntington, "The Elastic constants of Crystals. Solid State Physics" Vol. 7, p. 276, Academic Press, 1958.
14. R. M. Martin, Phys. Rev. B1, 4005, 1970.
15. G. E. Zardras, Thesis, Athens, 1983.