Acta Cryst. (1976). A32, 306

Internal Strain of GaAs. II. Transverse Case

BY C. N. KOUMELIS, G. E. ZARDAS, C. A. LONDOS AND D. K. LEVENTOURI

Department of Physics, University of Athens, Athens 144, *Greece*

(*Received* 7 *October* 1975; *accepted* 9 *October* 1975)

The effect of internal strain in the zincblende structure was examined on a GaAs single crystal by X-ray intensity measurements under a uniaxial stress along the [1$\bar{1}$0] direction. It was found that the stress changes the structure factor of the weak reflexion (006), giving the value $\zeta = 0{\cdot}764 \pm 0{\cdot}009$ for the bond-bending constant.

Introduction

In a previous paper (Koumelis & Rozis, 1975), the longitudinal case, *i.e.* the case in which the internal strain vector **u** is antiparallel to the macroscopic strain vector, was examined experimentally for GaAs. When a crystal of the zincblende structure is stressed along one of the ⟨110⟩ directions, the internal strain vector **u** is perpendicular to the direction of the stress (Segmüller & Neyer, 1965) (Fig. 1). This case can be described as the transverse case.

Calculations

The position vectors ϱ_j and $\mathbf{r}_j$ ($j=1,2,3,4$) of the four atoms of Ga and As in the cubic cell become under a uniaxial stress τ

$$\varrho_j' = \varrho_j\,, \quad \mathbf{r}_j' = (1+\varepsilon)\,.\,\mathbf{r}_j + \mathbf{u}\,,$$

where ε is the strain tensor and $\mathbf{u}(u_x, u_y, u_z)$ the vector of internal strain.

The reciprocal lattice vector $\mathbf{H}(h,k,l)$ in the strained crystal will be

$$\mathbf{H}' = \mathbf{H}\,.\,(1+\varepsilon)^{-1}.$$

Hence

$$\mathbf{H}'\,.\,\mathbf{r}_j' = \mathbf{H}\,.\,(1+\varepsilon)^{-1}\,.\,[(1+\varepsilon)\,.\,\mathbf{r}_j + \mathbf{u}] \simeq \mathbf{H}\,.\,\mathbf{r}_j + \mathbf{H}\,.\,\mathbf{u}\,.$$

The structure factor of the strained cell will be

$$F^{(\mathbf{u})}_{(hkl)} = f_{\mathrm{Ga}} \sum_1^j \exp\,(2\pi i \mathbf{H}\,.\,\varrho_j) + f_{\mathrm{As}} \sum_1^j \exp\,[2\pi i(\mathbf{H}\,.\,\mathbf{r}_j + \mathbf{H}\,.\,\mathbf{u})]\,.$$

For a weak reflexion, the above relation becomes

$$F^{(\mathbf{u})}_{(hkl)} = 4[f_{\mathrm{Ga}} - f_{\mathrm{As}} \exp\,(2\pi i \mathbf{H}\,.\,\mathbf{u})]\,.$$

The ratio of the integrated intensity of the strained and unstrained cell is

$$\frac{J^{(\mathbf{u})}_{(hkl)}}{J_{(hkl)}} = \frac{F^{(\mathbf{u})}_{(hkl)}\,F^{(\mathbf{u})*}_{(hkl)}}{F_{(hkl)}\,F^{*}_{(hkl)}} = \frac{f^2_{\mathrm{Ga}} + f^2_{\mathrm{As}} - 2f_{\mathrm{Ga}}f_{\mathrm{As}} \cos\,(2\pi \mathbf{H}\,.\,\mathbf{u})}{(f_{\mathrm{Ga}} - f_{\mathrm{As}})^2}\,.$$

The relative change of the integrated intensity is

$$\frac{\Delta J_{(hkl)}}{J_{(hkl)}} = \frac{J^{(\mathbf{u})}_{(hkl)} - J_{(hkl)}}{J_{(hkl)}} = \frac{4f_{\mathrm{Ga}}f_{\mathrm{As}}}{(f_{\mathrm{Ga}} - f_{\mathrm{As}})^2} \sin^2\,(\pi \mathbf{H}\,.\,\mathbf{u})\,. \tag{1}$$

The vector $\mathbf{u}(u_x, u_y, u_z)$ according to Segmüller & Neyer (1965) is

$$\begin{pmatrix} u_x \\ u_y \\ u_z \end{pmatrix} = -\frac{\zeta}{4} s_{44}\tau \begin{pmatrix} \alpha_2\,\alpha_3 \\ \alpha_3\,\alpha_1 \\ \alpha_1\,\alpha_2 \end{pmatrix},$$

where $\alpha_1, \alpha_2, \alpha_3$ are the direction cosines of τ. For τ along the [1$\bar{1}$0] direction

$$u_x = 0\,, \quad u_y = 0\,, \quad u_z = \frac{\zeta}{8} s_{44}\tau\,.$$

Hence, (1) for the reflexion 006 gives

$$\frac{\Delta J_{(006)}}{J_{(006)}} = 2{\cdot}25 \frac{f_{\mathrm{Ga}}f_{\mathrm{As}}}{(f_{\mathrm{Ga}} - f_{\mathrm{As}})^2} \pi^2\zeta^2 s^2_{44}\tau^2.$$

It is evident that, for a given τ, the ratio $\Delta J_{(006)}/J_{(006)}$ for the transverse case is 2·25 times larger than the longitudinal case (Koumelis & Rozis, 1975).

Results

The experimental procedure is the same as in Part I but Co $K\alpha$ radiation was used. Fig. 2 gives the integrated intensity of the 006 line *versus* τ. The statistical error for each point was 0·5% in the background,

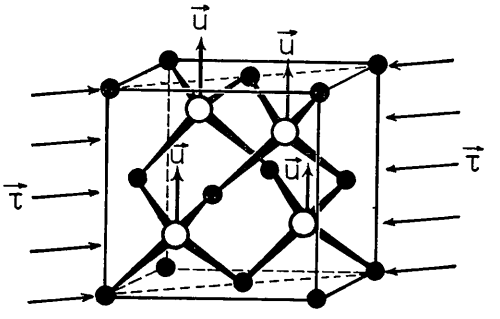

Fig. 1. Transverse case of the internal strain.

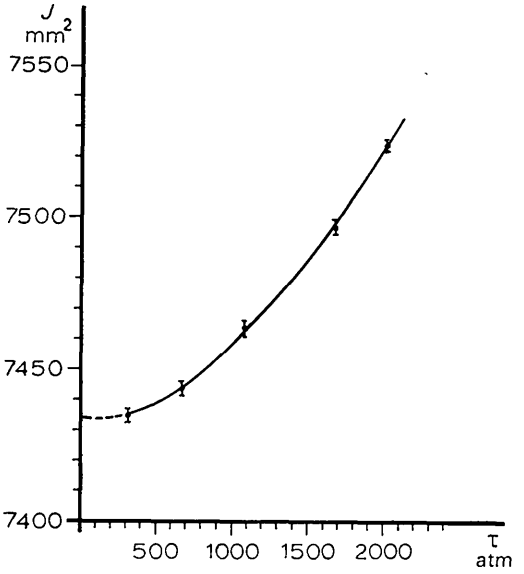

Fig. 2. Integrated intensity of the 006 line as a function of stress.

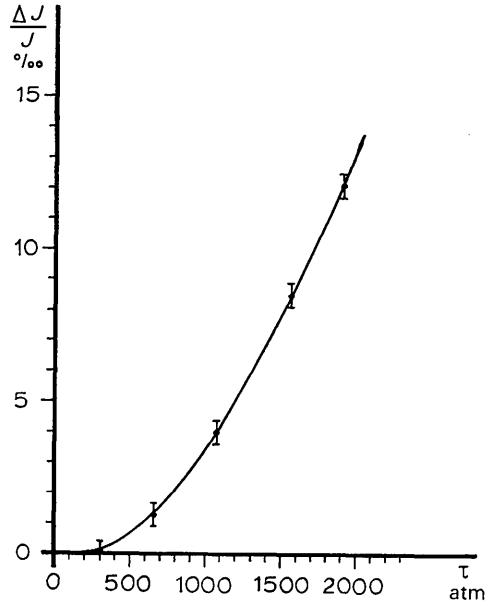

Fig. 3. Relative change of the integrated intensity *versus* τ.

and 0·2% in the peak. The crystal was fastened to the press with an initial stress of 315 atm. The integrated intensity corresponding to $\tau=0$ was found by extrapolation. Fig. 3 shows the ratio $\Delta J_{(006)}/J_{(006)}$ *versus* stress.

For the calculation of the bond-bending constant ζ, one has to choose values for the atomic scattering factors of Ga and As. The values given in various tables are valid for free atoms, whereas our measurements concern atoms in a solid. As no values are available for solids, we have to use those for free atoms for which however there is no criterion about the best approximation to solids (Weiss, 1975). According to Cromer (1965), the elements under discussion are in the region where the best approximation for free atoms is computed from variational wave functions (*International Tables for X-ray Crystallography*, 1962).

Table 1. *Experimental values of the bond-bending constant*

τ (atm)	ζ	$\delta\zeta$	$\delta\zeta/\zeta$ (%)
315	0·4	0·6	150
667	0·7	0·1	15
1080	0·78	0·04	5
1570	0·78	0·02	3
1914	0·76	0·014	2

For the elastic coefficient s_{44} of GaAs, the value $1{\cdot}6921\times 0^{-12}$ cm^2 dyn^{-1} was used (Cottam & Saunders, 1973). Table 1 gives the experimental values of ζ. Considering all the values of ζ with their weights according to their errors, we obtain the following mean value for ζ and the ratio α/β of the force constants

$$\zeta=0{\cdot}764\pm 0{\cdot}009\,,\quad \alpha/\beta=1{\cdot}21\pm 0{\cdot}01\,.$$

The value $\zeta=0{\cdot}764$ is in good agreement with the value $\zeta=0{\cdot}77$ found for the longitudinal case (Koumelis & Rozis, 1976). The present X-ray method gives a bond-bending constant larger by 12% than that calculated from elastic constants and transverse effect charge data (Martin, 1972).

References

Cottam, R. I. & Saunders, G. A. (1973). *J. Phys. C*, **6**, 2105–2118.

Cromer, D. T. (1965). *Acta Cryst.* **19**, 224–227.

International Tables for X-ray Crystallography. (1962). Vol. III, pp. 204–206.

Koumelis, C. N. & Rozis, E. I. (1975). *Acta Cryst.* A**31**, 84–88.

Koumelis, C. N. & Rozis, E. I.(1976). *Acta Cryst.* A**32**, 170.

Martin, R. M. (1972). *Phys. Rev.* B**5**, 1607–1613.

Segmüller, A. & Neyer, H. R. (1965). *Phys. Cond. Matter*, **4**, 63–70.

Weiss, R. J. (1975). Private communication.