$$X = 2|F||F_H|/\Sigma f_L^2\,.$$

It follows that

$$\frac{\text{Probability of } \alpha_1 \text{ being correct choice}}{\text{Probability of } \alpha_2 \text{ being correct choice}} = \frac{\exp\,[X \cos\,(\alpha_1 - \alpha_H)]}{\exp\,[X \cos\,(\alpha_2 - \alpha_H)]}$$

and the terms in the Fourier series representing the 'best' electron-density distribution are of the form

$$w|F|\,\exp\,(i\alpha_1) + (1-w)|F|\,\exp\,(i\alpha_2)\,,$$

where

$$w = \frac{\exp\,[X \cos\,(\alpha_1 - \alpha_H)]}{\exp\,[X \cos\,(\alpha_1 - \alpha_H)] + \exp\,[X \cos\,(\alpha_2 - \alpha_H)]}\,.$$

When the crystal contains only one type of anomalous scatterer the phase solutions α_1 and α_2 are most conveniently expressed (Ramachandran & Raman, 1956) as

$$\alpha_1 = \alpha_H + \pi/2 - \theta$$
$$\alpha_2 = \alpha_H + \pi/2 + \theta$$

where θ can be calculated in a direct manner from the Bijvoet inequality $\Delta|F|^2$. It can then be shown that

$$w = [1 + \exp\,(-2X \sin\,\theta)]^{-1}.$$

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Double Bragg scattering of X-rays in irradiated beryllium oxide.

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Double Bragg scattering of X-rays occurs when two or more reciprocal lattice points intersect the Ewald sphere so that the once-reflected beam is diffracted by a second set of planes. This produces a reflexion which is forbidden by normal space group considerations. This phenomenon, previously observed in substances like diamond (Renninger, 1937) and germanium (Cole, Chambers & Dunn, 1962), has now been detected in beryllium oxide during a study of the effects of neutron irradiation.

As BeO has the wurtzite structure the forbidden reflexions within the Cu $K\alpha$ sphere are those $hh\overline{2h}l$ reflexions for which $l = 2n+1$. The crystal examined was a thin flake of basal plane habit, which had been irradiated to a dose of $2{\cdot}5 \times 10^{20}$ nvt at 75 – 100 °C (> 1 MeV). A Buerger precession photograph of the $h0l$ reciprocal lattice plane showing the forbidden 001 reflexions as well as pronounced streaking along the reciprocal lattice rods $10l$, $20l$. The streaking can be satisfactorily explained in terms of extrinsic stacking faults in the (001) planes of the hexagonal lattice (Sabine, 1964). However, it seemed unreasonable that sharp superlattice reflexions could be produced by irradiation.

A more detailed investigation was subsequently made with a General Electric Goniostat and a proportional counter. Reflexions 001, 003, 005, as well as 111 and 113 were detected. The intensity distribution of the forbidden 001 reflexions was examined by rotating the crystal about the respective scattering vectors of the reflecting planes. A series of peaks was observed, which repeated every 60° of azimuth and was symmetrical about the midpoint of each range. The reflexions were identified by calculation of the crystal settings which gave rise to simultaneous intersection of the Ewald sphere by two reciprocal lattice points. When one of these reflexions was itself forbidden, no peak was observed. The results of this examination are shown in the Table 1.

The azimuthal position of the multiple scattering peaks is rather sensitive to a change in lattice parameters. Significant shifts from some of the unirradiated peak positions were observed and calculation showed that within the limits of experimental error these fitted the lattice parameters reported by Walker, Mayer & Hickman (1964).

The crystal was then annealed for one hour at 1400 °C, at which temperature other techniques indicate that irradiation damage effects disappear (Hickman & Pryor, 1964). Reflexions resulting from planes with high indices could now be detected. This is in accordance with other X-ray diffraction studies (Walker, Mayer & Hickman, 1964) in which it has been found that the higher the ratio $l^2 : h^2 + hk + k^2$ for a given reflexion, the greater is the radiation-induced broadening. Identical measurements were carried out on an unirradiated crystal of similar habit. Double Bragg scattering was also observed in this crystal and was comparable in intensity with that of the irradiated crystal annealed at 1400 °C.

To ensure that recovery of irradiation damage was complete, the crystals were annealed at 1600 °C. In both cases, the intensity of the forbidden reflexions increased, the increase being more noticeable for the irradiated crystal. The reason for this increase is not known. It seems more probably due to recovery of imperfections introduced during growth than to further recovery of irradiation damage.

It has been shown by other techniques (Sabine, Pryor

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* Attached from South African Atomic Energy Board.

Table 1. *Multiple scattering peaks for forbidden* 001 *reflexions*

Azimuth (°)	Reflecting planes		Irradiated specimen 2×10^{20} nvt (c.sec^{-1})	1 hr annealed 1400 °C (c.sec^{-1})	1600 °C (c.sec^{-1})	Control specimen (c.sec^{-1})	1 hr annealed 1600 °C (c.sec^{-1})
	001 Reflexion						
5·2	$10\bar{1}2$	$10\bar{1}3$	54	640	1550	500	430
10·0	$20\bar{2}2$	$20\bar{2}1$	18	40	120	75	56
13·1	$20\bar{2}2$	$20\bar{2}3$		120	270	170	120
16·8	$21\bar{3}1$	$21\bar{3}0$	25	36	160	50	80
18·1	$20\bar{2}0$	$20\bar{2}1$	20	40	225	40	85
19·6	$10\bar{1}1$	$10\bar{1}0$	250	260	1600	180	450
21·4	$12\bar{3}1$	$12\bar{3}0$	25	33	155	60	60
27·4	$12\bar{3}2$	$12\bar{3}1$		30	85	50	35
28·4	$10\bar{1}2$	$10\bar{1}1$	162	310	1250	250	230
	003 reflexion						
3·9	$10\bar{1}1$	$10\bar{1}4$		14	34	8	5
8·4	$21\bar{3}2$	$21\bar{3}1$		20	57	25	16
8·9	$20\bar{2}0$	$20\bar{2}3$		35	120	30	15
9·4	$10\bar{1}2$	$10\bar{1}1$	54	175	570	100	121
18·3	$20\bar{2}1$	$20\bar{2}2$		7	17	8	5
22·8	$10\bar{1}3$	$10\bar{1}0$	35	160	680	60	112
26·0	$20\bar{2}1$	$20\bar{2}4$		4	20	6	5
29·7	$12\bar{3}2$	$12\bar{3}1$		22	60	20	20
	005 reflexion						
5·6	$1\bar{1}01$	$1\bar{1}04$		6	15	3	3
7·5	$20\bar{2}2$	$20\bar{2}3$		44	84	27	20
16·2	$10\bar{1}0$	$10\bar{1}5$	6	83	480	30	100
22·7	$20\bar{2}4$	$20\bar{2}1$		5	13	4	4
29·6	$1\bar{1}03$	$1\bar{1}02$	17	320	500	63	90

& Hickman, 1963) that the defect concentration in BeO at $2{\cdot}5\times10^{20}$ nvt (> 1 MeV) is approximately 1·5% and that these defects are present in clusters approximately 50 Å in diameter. The present experiments show that this defect concentration does not destroy the perfection of the crystal sufficiently for double Bragg scattering effects to disappear.

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La polarité de la liaison carbonyle et la structure cristalline de l'alloxane, de l'acide barbiturique anhydre et des composés analogues.

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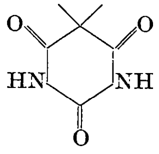
L'étude de la structure cristalline de certains composés polycarbonylés tels, en particulier, l'acide parabanique (I) (Davies & Blum, 1955), l'acide barbiturique anhydre (II) (Bolton, 1963) et l'alloxane (III) (Bolton, 1964) a permis de mettre en évidence l'existence dans ces cristaux d'approches intermoléculaires particulièrement réduits entre les oxygènes de certains carbonyles et certains carbones du cycle. Cette particularité ne paraît pas se retrouver dans la structure cristalline d'autres bases pyrimidiques ou puriques d'intérêt biologique. Bolton (1964) attribue cet état de choses à la polarité exceptionnellement prononcée des groupes carbonyles impliqués dans les contacts rapprochés. Cet auteur observe toutefois en même temps, que les liaisons en question sont exceptionnellement courtes.

(I)



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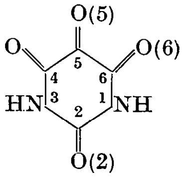

(III)