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The Crystal Structure of the β Phase of Uranium

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The crystal structure of the β phase of metallic uranium (stable between 660 and 760° C.) has been deduced from X-ray diffraction measurements made on single crystals of the phase retained in an alloy containing 1·4 atomic % chromium and rapidly cooled from 720° C. The diffraction data and other measurements show that the unit cell of the β phase is tetragonal, with $a_0 = 10{\cdot}52$, $c_0 = 5{\cdot}57$ A., and contains 30 atoms. Of the three possible space groups (*P*4/*mnm*, *P*4*nm* and *P*$\bar{4}$*n*2), *P*4/*mnm* appears definitely excluded, while of the remaining two, *P*4*nm* appears to account adequately for the diffraction intensities. Positions of the 30 atoms in the unit cell have been deduced using the Patterson and Patterson–Harker F^2 syntheses and the Fourier electron-density synthesis.

The β phase has a layer structure with the layers parallel to the a_0b_0 plane of the unit cell at $\frac{1}{4}c_0$ and $\frac{3}{4}c_0$. Midway between the layers are atoms which are linked to those in the adjacent layers but not to each other. The layers are quite closely related to the basal planes of the familiar hexagonal close-packed structure, except that atoms at the centers of certain hexagons are displaced normal to the layers to form the set of atoms found midway between the layers. A structure essentially the same as that of β uranium is being found by other investigators for the σ phase of the Fe–Cr and other systems.

The low symmetry and complexity of the structure accounts for the rather hard, brittle nature of the phase. The interrelations between the α, β and γ phases of the metal are clear from the β-phase crystal structure, but the precise mechanism of the transformations has not yet been studied.

Introduction

It is now well known that the element uranium exhibits three crystalline modifications. The α phase is stable from ordinary temperatures up to 660° C., the β phase from 660 to 760° C., and the γ phase from 760° C. to the melting-point.

The crystal structure of the α phase was determined by Jacob & Warren (1937) and that of the γ phase was first published in the unclassified literature by Wilson & Rundle (1949). The α phase is orthorhombic having lattice parameters $a_0 = 2{\cdot}852$, $b_0 = 5{\cdot}865$ and $c_0 = 4{\cdot}945$ A. The γ phase is body-centered cubic with $a_0 = 3{\cdot}474$ A. at room temperature.

Some work on the β phase was carried on at Iowa State College and at the Battelle Memorial Institute during the past ten years. The work consisted of obtaining powder patterns of the metal at high temperatures and of the phase retained at room temperature in alloys quenched from the β region and containing several atomic % chromium or molybdenum. The powder patterns so obtained did not yield to analysis owing to their complexity. Similar work was carried on at the Knolls Atomic Power Laboratory by the present author (Tucker, 1950*a*), and similar results were obtained.

Unit cell and space group of the β phase

More recently single crystals of the β phase have been made by lowering a uranium wire containing 1·36 atomic % chromium through a thermal gradient into the β region and quenching in water. Laue, rotation and Weissenberg patterns of such a single crystal established that the unit cell was tetragonal. Refinement of the unit-cell dimensions, using powder and single-crystal pattern data, gave the values

$$a_0 = 10{\cdot}52, \quad c_0 = 5{\cdot}57 \text{ A.}$$

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From the density of the alloy (18·697 g.cm.$^{-3}$), its composition, and the unit-cell dimensions, the number of atoms per unit cell was found to be 30.

The only space-group extinctions present in the single-crystal data were $0kl$ present only when $k+l=2n$ (and, of course, $h0l$ present only when $h+l=2n$), thus revealing the presence of a diagonal glide plane. The three tetragonal space groups with this extinction are $P4/mnm(D_{4h}^{14})$, $P4nm(C_{4v}^{4})$ and $P\bar{4}n2(D_{2d}^{8})$. The space group $P4/mnm$ appears to be ruled out on the basis of intensity considerations to be mentioned later. Thus far, $P4nm$ is adequate to account for the diffraction intensities. $P\bar{4}n2$ has not been considered in great detail.

Location of the atoms in the unit cell

Because the unit cell of the β phase is relatively flat the most fruitful approach to the problem of locating the 30 atoms in the unit cell was to obtain an $a_0 b_0$ projection of the structure. To this end a single crystal was oriented to rotate about the fourfold axis, and a rotation pattern and Weissenberg patterns of the 0, 1, 2 and 3 levels were obtained. In obtaining the Weissenberg patterns four films were placed in series and exposed for 64 hr. using filtered copper $K\alpha$ radiation, an X-ray tube potential of 35 kV., and a filament current of 20 mA. As nearly as possible the tube current and potential, and the film development conditions for each set of four films were maintained constant. The intensities on these films were estimated by comparison of the reflection densities with those on a piece of strip film (of the same type) on which areas had been exposed to X-rays of the same quality for various lengths of time. The factor to be applied in correcting the intensities of the reflections for absorption by various layers of film was obtained by densitometer measurements on four strip films which had also been placed in series. Correction of the intensity values for absorption, temperature, Lorentz and polarization factors, and extinction was not attempted because the absorption correction for the crystal in its initial form would have been very difficult to make owing to its geometry. Also it is compensated to some extent by the Lorentz and polarization factors in the region of low-order reflections. While it was realized that the intensity values left something to be desired, it was felt that they would not be grossly in error and would permit an unambiguous structure determination in a minimum amount of time.

As a first step the Patterson projection on the $a_0 b_0$ plane was calculated, using the $hk0$ intensities (Fig. 1)*. Although the figure shows only one-fourth of the unit cell, the remainder may be obtained by symmetry considerations. Interpretation of this figure by itself would be a difficult matter for a unit cell containing 30 atoms of high atomic number. The occurrence of a number of large well-resolved peaks was, however, informative. These peaks are seen to fall on the 45° line and on lines of slopes approximately $\frac{1}{4}$ and 4.

Next, the Patterson–Harker $a_0 b_0$ section was calculated and is shown in Fig. 2, once more only one-fourth of the unit cell being given. On comparing Figs. 1 and 2, one notices immediately their similarity, the major maxima along the 45° line and along lines of slope $\frac{1}{4}$ and 4 occurring in almost precisely the same positions. This suggested that the structure consisted of layers lying parallel to the $a_0 b_0$ plane. Upon examining space group $P4/mnm$ it was clear that a Patterson–Harker section along the line $\frac{1}{2}, y, \frac{1}{2}$ would give the atomic co-ordinates directly, or at least simple linear functions of them. This section was therefore calculated. The resulting curve (Fig. 3) shows four well-resolved maxima with a fifth occurring as a shoulder on the fourth at the extreme right. Owing to ambiguities inherent in the method each maximum can correspond to one or more of four values for atomic parameters. Fortunately, however, detailed examination of these atomic parameters eliminated all save one or possibly two sets. Substitution of the most likely set of atomic parameters into a simplified form of the equation for the structure factor for the space group $P4/mnm$, taken from the *Internationale Tabellen...* (1935), gave qualitatively correct values for the strongest $hk0$ intensities. Taking the signs of the calculated structure factors for the strongest $hk0$ reflections and the square roots of their observed intensities, an $hk0$ Fourier summation of the electron density was calculated using the equation given by Lonsdale (1936) for the space group $P4/mnm$. The result is shown in Fig. 4. The agreement between the assumed atomic positions shown by the crosses and the peaks in the electron-density function is seen to be quite good.

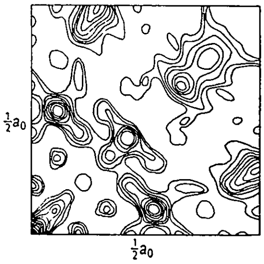

Fig. 1. Patterson $hk0$ projection.

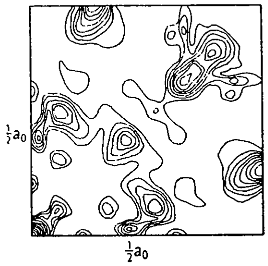

Fig. 2. Patterson–Harker $hk0$ section.

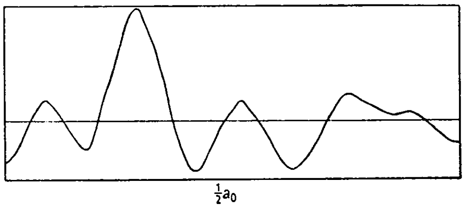

Fig. 3. Patterson–Harker section at $\frac{1}{2}$, y, $\frac{1}{2}$.

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* The Patterson, Patterson–Harker, and Fourier syntheses here reported were calculated using the well-known Beevers–Lipson strips. The set used gave values at 6° intervals.

The atomic positions shown in Fig. 4 suggested immediately a possible structure for the β phase. The figure shows that surrounding each of four of the peaks in the projection are 12 atoms. Dividing these into two groups of six each, each group of six forms a hexagon, thus producing two layers of atoms with triangular close-packing within each layer. An additional feature of this arrangement was that the interatomic distances for atoms within and between layers all fell between 2·66 and 3·27 A. It will be recalled that the interatomic distances found in the α phase are 2·76, 2·85, 3·26 and 3·32 A., while in the γ phase the single value of 3·00 A. occurs. Thus the interatomic distances for the postulated β-phase structure were entirely within the bounds to be expected. The structure also gave 30 atoms per unit cell in agreement with the value given by lattice-parameter and density measurements. Calculation of a number of *hkl* intensities, using the structure factor for the space group $P4/mnm$ and the z parameters of the postulated layer structure, however, gave clearly incorrect results in a number of cases, so this postulated structure had to be abandoned, although the final structure is not greatly different from it.

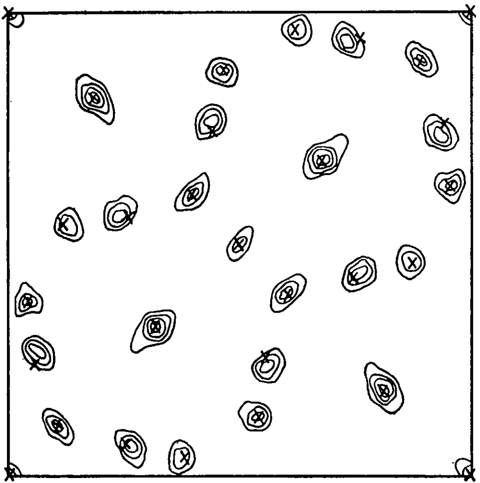

Fig. 4. Fourier *hk*0 projection.

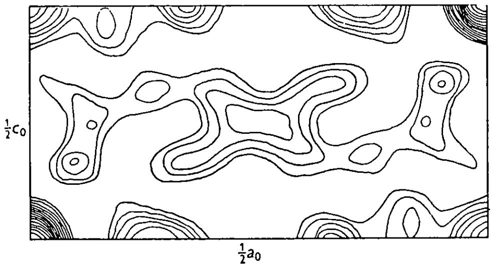

Fig. 5. Patterson 0*kl* projection.

To obtain some indication of the values for the z parameters a Patterson 0*kl* projection was calculated (Fig. 5). This showed immediately that while there were quite possibly atoms at $z=0{\cdot}00$ and $0{\cdot}50$, there were a number with z parameters in the neighborhood of $z=0{\cdot}25$ and $0{\cdot}75$. A study of the 0*kl* Patterson projection made it possible to deduce the z parameters of a number of the atoms. Using these x, y and z parameters and a simplified form of the structure factor from the *Internationale Tabellen*...(1935) for the space group $P4nm$[*] (that of next highest symmetry below $P4/mnm$), the phases of the strongest *hkl* reflections were calculated. With these phases and the square roots of the observed intensities for the absolute values of the structure factors, a Fourier 0*kl* projection of the structure was calculated, using a simplified form of the equation for the electron-density function taken from the tables of Lonsdale (1936) for the space group $P4nm$. After several trials a third 0*kl* Fourier projection was calculated (Fig. 6). The crosses on this figure indicate the atomic positions upon which the calculation is based. The numerical values of the atomic position parameters are given in Table 1. It is seen from Fig. 6 that the crosses all fall quite close to major maxima in the figure, although some modification of the atomic positions is suggested. There are still several fairly large maxima, notably two in the lower left corner of the figure, which do not correspond to assumed atomic positions. Since such maxima have been reduced from larger values in the first two projections, it seems probable that these will be eliminated upon further refinement of the parameters.

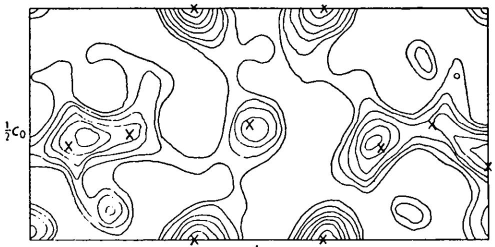

Fig. 6. Fourier 0*kl* projection.

Table 1. *Atomic parameters based on space group P4nm*

2 atoms in (*a*)[*]			$z=0{\cdot}66$
4 atoms in (*c*)	$x=0{\cdot}11$,		$z=0{\cdot}23$
4 atoms in (*c*)	$x=0{\cdot}32$,		$z=0{\cdot}00$
4 atoms in (*c*)	$x=0{\cdot}68$,		$z=0{\cdot}50$
8 atoms in (*d*)	$x=0{\cdot}56$,	$y=0{\cdot}24$,	$z=0{\cdot}25$
8 atoms in (*d*)	$x=0{\cdot}38$,	$y=0{\cdot}04$,	$z=0{\cdot}20$

[*] Positions given in *Internationale Tabellen*...(1935) under space group C_{4v}^4 on page 184.

With the rather good agreement between assumed atomic positions and the calculated *hk*0 and 0*kl* Fourier electron-density projections, the absolute values of the structure factors for all *hkl* reflections, based on the space group $P4nm$ and the atomic positions in Table 1,

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[*] Changing to this space group did not affect the previous work on the x and y atomic parameters or the *hk*0 projection of the structure because the two space groups are equivalent as regards the *hk*0 projection. The change in space groups was dictated by detailed intensity considerations.

Table 2. *Comparison of* $|F|_c$ *with* $|F|_o$

		$l=0$		$l=1$		$l=2$		$l=3$	
h	k	$\|F\|_c$	$\|F\|_o$	$\|F\|_c$	$\|F\|_o$	$\|F\|_c$	$\|F\|_o$	$\|F\|_c$	$\|F\|_o$
1	0	0	0	3	0	0	0	0	3
1	1	1	0	1	0	7	3	4	3
2	0	1	0	0	0	19	10	0	0
2	1	0	0	3	0	22	10	10	0
2	2	0	0	2	0	16	7	5	3
3	0	0	0	2	0	0	0	4	4
3	1	4	0	5	4	8	10	7	3
3	2	1	0	3	3	5	4	5	0
3	3	30	71	28	22	9	3	27	17
4	0	10	3	0	0	5	3	0	0
4	1	29	71	26	35	3	4	24	22
4	2	3	3	9	0	2	1	9	3
4	3	3	0	6	4	5	4	5	3
4	4	4	5	5	2	2	2	4	3
5	0	0	0	9	1	0	0	4	3
5	1	6	5	8	4	9	7	10	8
5	2	1	5	1	3	13	17	2	1
5	3	0	5	1	0	9	17	1	0
5	4	6	5	7	4	14	4	10	2
5	5	27	17	22	22	8	3	20	22
6	0	0	2	0	0	30	17	0	0
6	1	1	2	3	1	14	17	7	1
6	2	7	7	8	6	9	17	8	3
6	3	1	5	3	3	9	7	7	9
6	4	1	5	5	7	4	7	4	4
6	5	12	7	3	0	4	1	3	5
6	6	28	17	25	22	4	3	24	22
7	0	0	0	6	6	0	0	8	4
7	1	5	2	2	2	4	3	4	2
7	2	37	41	17	22	13	10	13	17
7	3	1	2	5	5	3	3	5	2
7	4	0	7	3	1	30	32	8	1
7	5	1	2	6	5	2	3	8	9
7	6	7	7	8	7	8	10	6	5
7	7	0	0	4	6	5	0	11	17
8	0	2	3	0	0	26	17	0	0
8	1	1	1	4	2	9	3	7	3
8	2	34	41	14	22	14	10	13	9
8	3	6	0	3	2	3	2	2	8
8	4	2	3	5	7	10	2	6	9
8	5	7	1	10	7	1	3	8	4
8	6	8	10	11	4	16	10	12	4
8	7	4	3	7	5	9	7	11	5
8	8	2	2	6	3	27	32	6	3
9	0	0	0	13	3	0	0	17	5
9	1	1	2	6	3	7	7	6	0
9	2	10	7	13	4	7	5	11	5
9	3	0	1	2	0	23	17	7	1
9	4	3	1	2	1	20	17	5	0
9	5	16	10	4	1	3	4	4	1
9	6	22	32	17	24	11	10	14	22
9	7	10	10	6	4	10	7	5	1
9	8	9	10	4	1	3	2	8	5
9	9	38	71	9	9	20	20	—	—
10	0	2	3	0	0	13	7	0	0
10	1	12	7	14	3	16	7	15	3
10	2	6	1	2	0	10	4	5	3
10	3	1	5	6	7	7	2	7	5
10	4	2	5	2	1	8	3	7	5
10	5	29	32	18	22	11	5	15	22
10	6	16	10	5	1	6	1	5	5
10	7	1	5	3	2	28	32	1	4
10	8	2	1	6	4	6	7	—	—
10	9	17	22	—	—	—	—	—	—
11	0	0	0	7	0	0	0	7	3
11	1	26	22	18	6	13	10	17	8
11	2	6	3	9	3	4	2	6	0
11	3	13	10	13	3	16	10	13	4
11	4	1	2	7	3	4	0	8	5
11	5	12	10	4	3	20	10	8	8
11	6	2	1	4	3	4	3	—	—
11	7	0	1	6	7	—	—	—	—
12	0	2	1	0	0	19	7	0	0
12	1	13	7	13	3	11	7	11	7
12	2	4	1	0	2	6	5	1	7
12	3	21	22	15	7	14	17	—	—
12	4	7	5	3	3	11	5	—	—
12	5	0	10	8	5	—	—	—	—
12	6	12	10	—	—	—	—	—	—

were calculated and compared with the square roots of the observed intensities. The results of these calculations are given in Table 2. Since the intensities of X-ray reflections are such sensitive functions of atomic positions and the atomic parameters are not completely refined, it is felt that the agreement shown is quite satisfactory. All major maxima in the diffraction pattern are found in the calculated values to be large. Also there are no large maxima found in the calculated values for which the observed value is low. Among the reflections of moderate and lesser intensity there is rather naturally, in many cases, poor agreement. This is to be expected in a structure for which the atomic position parameters are not completely refined, as the intensities of the weaker reflections are more sensitive to changes in atomic parameters than are those of the strong reflections. Of special interest is a series of reflections of the type 930, 931, 932 and 933 or 940, 941, 942 and 943. In these cases the reflections with $l=0$, 1 and 3 are all weak, whereas the values for $l=2$ are large. These changes are reflected in the calculated values. Similar effects occur, for example, in the set 410, 411, 412 and 413, for which the reflection for $l=2$ is weak while the other three are strong. Cases of agreement such as these, which occur repeatedly, do much to confirm the correctness of the structure because such variations in intensity were not built into the structure, in the sense that the Patterson and Fourier projections used only the $hk0$ and $0kl$ intensities and not the hkl values. It is true that the Patterson–Harker $hk0$ and $\frac{1}{2}, y, \frac{1}{2}$ sections did use all intensities, but these used sums of groups of intensities which would not contain variations of the type discussed here.

Discussion of the structure

The crystal structure of the β phase may be regarded essentially as a layer structure. The layers, not perfectly flat but reasonably so, occur at $z=0{\cdot}25$ and $0{\cdot}75$. These layers are fixed in position by contact of atoms in a given layer with atoms in adjacent layers and also by contact with atoms midway between the layers at $z=0{\cdot}00$, $0{\cdot}50$ and $1{\cdot}00$. These latter atoms form a layer of the type shown in Fig. 7 (layer of type A). This A-type layer is not self-supporting because the atoms within the layers are not in contact with one another. The A-type layers are separated by 2·79 A. and form continuous rows of atoms throughout the structure parallel to c_0.

Midway between the A-type layers are layers of types B and C (Figs. 8, 9). The B-type layer occurs at $z=0{\cdot}25$ and the C type at $z=0{\cdot}75$. These two layers may be brought into coincidence by simple rotation and translation. The B- and C-type layers are separated by 2·79 A. and midway between them is an A-type layer. Thus the stacking order of the layers is $A\,B\,A\,C\,A\,B\,A\,C\ldots$.

The positions at the centers of the hexagons in the B- and C-type layers are unoccupied, but 1·39 A. above and below these positions there are atoms in A layers. The interatomic distances between the atoms in the A-type layers and the six corner atoms of the hexagons in the B- and C-type layers vary between 2·82 and

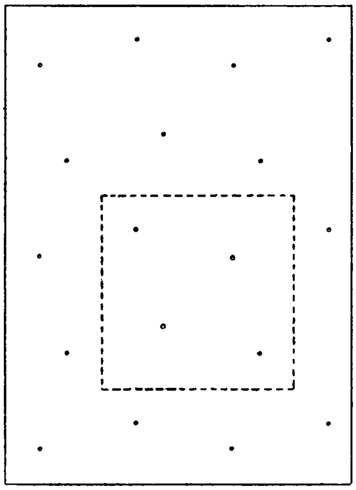
Fig. 7. A-type layer (unit cell shown by broken lines).

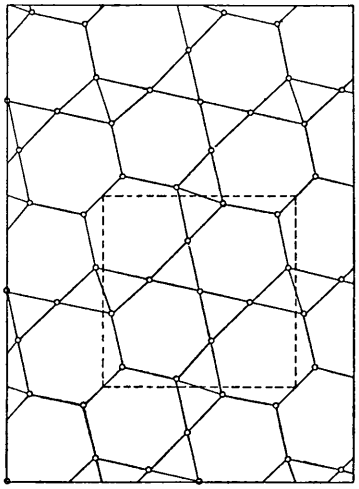
Fig. 8. B-type layer (unit cell shown by broken lines).

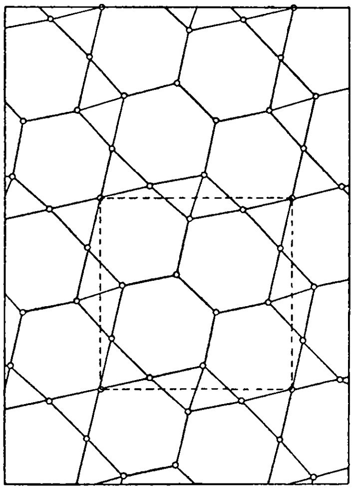
Fig. 9. C-type layer (unit cell shown by broken lines).

3·54 A. The interatomic distances within the *B*- and *C*-type layers vary between 2·66 and 3·27 A. A detailed study of the co-ordination of the atoms in the structure shows that the atoms have either 12, 14 or 15 nearest neighbors.

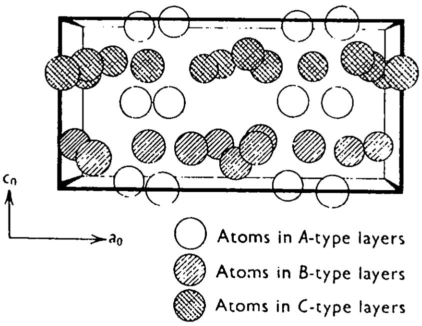

Fig. 10. View of unit cell showing layer structure.

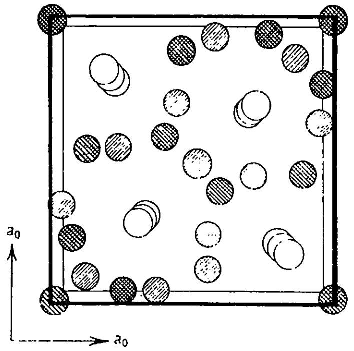

Fig. 11. View of unit cell along fourfold axis. Key as for Fig. 10.

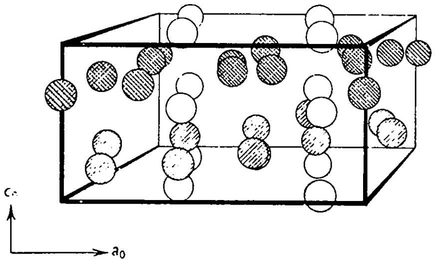

Fig. 12. View of unit cell along (410) planes. Key as for Fig. 10.

Various features of the structure may be seen in Figs. 10–12. The layer nature is readily seen in Fig. 10. Fig. 11 shows the open hexagons formed by the grey and black spheres in the *B*- and *C*-type layers, as well as the strings of white spheres (from atoms in the *A*-type layers) which go through the structure parallel to c_0. Fig. 12 shows a view along the (410) planes which are rather densely packed. The alignment of the spheres on these planes is evident.

Relation of the β- to the α- and γ-phase crystal structures

It is easy to see a connection between the β- and the α- and γ-phase crystal structures, but the mechanism of the transformations is not immediately obvious. By moving the *A*-type layers of the β-phase structure normal to themselves a distance of 1·39 A., their atoms fill the vacancies at the centers of the open hexagons in the *B*- and *C*-type layers. They then form triangular close-packed layers similar to the basal planes of the hexagonal close-packed structure, which, in a distorted form, supplies the basis for building the α- and γ-phase structures. Once the triangular close-packed sheets are formed from the β phase, however, considerable motion of the sheets would be necessary to form the α- and γ-phase structures. This makes such a simple approach seem unlikely. It is clear, however, from an examination of the β-phase structure that the transformations from the β- to the α- and γ-phase structures can be accomplished by small atomic motions, but the precise motions necessary have not yet been studied in detail.

Relation of the β-uranium structure to the σ-phase structure of the Fe–Cr and other systems

Since the β-uranium structure was reported (Tucker, 1950*b, c*), it has been discovered by Dickins, Douglas & Taylor (1951*a, b*) that the σ-phase structure found in the Fe–Cr and Co–Cr (and possibly other systems in which this phase occurs) is essentially the same as the β-uranium structure. A further independent check on this point is given by the work of Shoemaker & Bergman (1951), who have made an analysis of the σ-phase structure, obtaining essentially the same results as those reported here for the β-uranium structure. J. S. Kasper and co-workers (private communication) are also finding similar results for the σ phase. The fact that both β-uranium and the σ phase are rather hard and brittle fits in well with the very close similarity, if not identity, of their crystal structures.

Another interesting feature of the β-uranium structure is that a Brillouin polyhedron, deduced from the X-ray powder pattern, is very nearly tangent to the inscribed sphere containing six valence electrons per atom. The polyhedron is formed by the (522), (413), (550), (333), (720) and (004) planes, all of which give strong X-ray reflections. These planes combine to form a highly symmetrical Brillouin polyhedron. The presence of this zone boundary just outside the sphere of six states is the type of result quite frequently found in complex metallic crystal structures, suggesting that these structures are stabilized by the presence of a nearly full Brillouin zone.

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the structure which eventually led to the identification of the correct unit cell.

It is also a pleasure to acknowledge the benefit of the advice, discussion, and encouragement of Drs David Harker, John P. Howe and John R. Low, all of whom helped so much and are therefore mentioned alphabetically.

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Determination of Elastic Constants of Crystals from Diffuse Reflexions of X-rays. II. Application to some Cubic Crystals

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The formulae required to deduce the elastic constants of cubic crystals from observations of diffuse reflexions are derived from the general theory. The intensities of the diffuse reflexions corresponding to points in reciprocal space distributed along various lines are compared. These lines are always taken in pairs which pass through the same reciprocal-lattice point, e.g. 400, and are parallel to important crystallographic axes, e.g. [110], [111]. Comparisons of these diffuse intensities lead directly to a measurement of ratios of the three elastic constants c_{11}, c_{12}, c_{44}, with an accuracy of about 5 %. Absolute values can be determined from an absolute measurement of the diffuse intensity, though with a lower accuracy. The method was tested using crystals of KCl and KBr and found to give results in agreement with measurements by other methods. It was also applied to $NaClO_3$, galena PbS, and hexamethylenetetramine. The last crystal was chosen as an example of a soft organic crystal which could not easily be studied by other methods, and it is believed to be the first purely organic cubic crystal for which the elastic constants have been determined. The results obtained for these five crystals were as follows:

	c_{11}	c_{12}	c_{44}
KBr	$3{\cdot}8\times10^{11}$	$0{\cdot}60\times10^{11}$	$0{\cdot}64\times10^{11}$ dyne cm.$^{-2}$
KCl	4·3	0·75	0·79
$NaClO_3$	4·9	1·5	1·2
Galena	10·2	3·8	2·5
Hexamethylenetetramine	1·5	0·3	0·7

1. Introduction

In a previous paper (Ramachandran & Wooster, 1951) (hereafter referred to as I) the general principles of a new method were described, in which the elastic constants of crystals are derived from measurements of diffuse reflexion. In this paper it is proposed to describe the results of such measurements for certain cubic crystals. Five crystals have been studied: two alkali halides, KCl and KBr; two inorganic compounds, PbS and $NaClO_3$; and one organic crystal, hexamethylenetetramine, $C_6H_{12}N_4$. Of these, the elastic constants of KCl and KBr are known fairly accurately, and the present experiments with these crystals were performed to test the applicability of the principles described in the earlier paper. The elastic constants of the other three materials were either not known, or different observers had obtained differing results.

2. Some general formulae

We may briefly recapitulate the main definitions and formulae used in calculating the results. Any reciprocal-lattice point of indices *hkl* is known as the 'relp' *hkl*. Starting from this relp a line having direction ratios *A*, *B*, *C* may be drawn, and this is known as the 'rekha' $[ABC]_{hkl}$. The line joining the 'relp', *hkl*, to the origin is known as the corresponding 'rel-vector'. The ratio of the intensity of X-rays diffusely reflected per unit

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