and H arise from reflections from different crystal sections, E and G, there is no coherence between them, and no interference can be expected. It is only for the one incident ray, that which passes through the intersection of sheets B and E and which is *simultaneously* reflected by more than one plane, that interference effects are possible. This fact suggests two experimental approaches. Either one may employ a closely collimated incident beam, restricted to lie in one of the sheets B or E, and study the form of the maxima and minima in reflections when simultaneous reflection occurs (Williamson & Fankuchen, 1955, 1956), or one could use the present technique to study the fine-structure of intersections of extinction lines in the directly transmitted beam, attempting to do with X-rays what Miyake & Kambe have done for electrons (Kambe, 1954). In either case there are serious obstacles to be overcome, even supposing the techniques were developed to give adequate resolution. The volume of crystal traversed by the X-ray beam may be expected to contain many coherent domains, and the configuration of internal domain boundaries will be unknown. Hence the form and strength of the dispersion surface for each domain may be different, all effects observed would be the resultant of contributions from a number of domains, and could hardly be expected to be interpretable. Only if a sufficiently thin slice of a highly perfect crystal were used as specimen would there be a good possibility of obtaining defined boundary conditions. Unfortunately such crystals are not likely to be encountered among those for which it is a matter of practical interest to gain information on relative phases of reflections.

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The Crystal Structure of the Metallic Phase Mg_{32} (Al, Zn)$_{49}$*

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A complete determination of the crystal structure of the ternary phase (λ or T phase) in the magnesium–aluminum–zinc system with composition approximately $Mg_3Zn_3Al_2$ has been carried out with use of intensity data from single-crystal Weissenberg photographs. The refinement of the structural parameters was carried out by use of Fourier projections, followed by application of the method of least squares. The unit of structure, based on the body-centered cubic lattice, has $a_0 = 14{\cdot}16$ Å, as previously reported by Laves, Löhberg & Witte. The space group is T_h^5, with 162 atoms per unit cube. The structure shows the correct formula to be Mg_{32}(Al, Zn)$_{49}$; there is some disorder in occupancy of positions by aluminum and zinc atoms. The icosahedron and truncated tetrahedron are prominent coordination polyhedra in this structure.

Introduction

Phase diagram studies of the magnesium–aluminum–zinc system have shown that there exists a ternary phase, which has been given the name λ phase or T phase (Egar, 1913; Köster & Wolf, 1936; Köster & Dullenkopf, 1936; Riederer, 1936; Fink & Willey, 1937; Little, Raynor & Hume-Rothery, 1943). The approximate composition $Mg_3Zn_3Al_2$ was assigned to the phase, which extends over a wide range of values of the Zn/Al ratio. The atomic percentage of magnesium is nearly constant for the alloys, as would be expected from the fact that the metallic radius of magnesium is about 15% greater than those of aluminum and zinc.

Laves, Löhberg & Witte (1935) made an X-ray

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study of the phase, and reported that the structure is based on a body-centered cubic lattice with $a_0 = 14{\cdot}16 \pm 0{\cdot}03$ Å, the calculated number of atoms per unit cell being 161. They also found that the ternary phase with approximate composition Mg_4CuAl_6 described by Vogel (1919) has almost certainly the same structure; the value of a_0 for this phase was found to be $14{\cdot}25 \pm 0{\cdot}03$ Å, with 161 atoms per unit cube. Strawbridge, Hume-Rothery & Little (1947) reported the existence of a quaternary magnesium–aluminum–zinc–copper phase, including these two ternary regions. We have made an X-ray study of a representative crystal, containing magnesium, zinc, and aluminum, which has led to a complete structure determination. Brief accounts of the structure have been published (Bergman, Waugh & Pauling, 1952; Pauling, 1955). In the present paper the results of a refinement of the parameter values are communicated, together with a detailed discussion of the structure.

Experimental methods

Crystals of the phase were made by melting the pure metals in proportions corresponding to the composition $Mg_3Zn_3Al_2$ in a sealed quartz tube, mixing the melt by vigorous shaking, and then allowing it to solidify by slow cooling (about 10° C. per hour). The appearance of the quartz tube after the pellet had been removed indicated that there had been some reaction between the quartz and the melt; chemical analysis showed, however, that the crystals of the metallic phase did not contain more than 0·1 atomic % of silicon. A complete analysis gave the following result:

Mg, 22·1%; Zn, 60·8%; Al, 17·0%; Si, < 0·1%.

This composition is very nearly the composition $Mg_3Zn_3Al_2$.

Laue photographs of isolated single crystals about 0·1 mm. in diameter were found to have Laue symmetry T_h. Rotation and Weissenberg photographs verified the value of a_0 quoted by Laves *et al.* (1935). Visual estimates of intensities of reflections for planes *hk*0 were obtained from Weissenberg photographs (copper $K\alpha$ radiation) with use of the multiple-film techniques of Lange, Robertson & Woodward (1939) and Robertson (1943). Estimates of intensities of some general reflections *hkl* were also made. Powder photographs did not indicate the presence of a second phase.

Determination of the structure

No systematic extinctions were found in addition to those characteristic of body-centering. The only space groups with Laue symmetry T_h allowed by this observation are T_h^5, T^3, and T^5. No non-systematic absences were recorded.

A structure based upon space group T_h^5 has been derived by use of the stochastic method. The assumption was made that, in this crystal, as in a number of other metallic crystals containing atoms with metallic radii differing by about 15%—for example, those with composition A_2B_{11}:Mg_2Zn_{11} and $Mg_2Cu_6Al_5$ (Samson, 1949) and Na_2Cd_{11} (Pauling & Ewing)—the structure is based upon the ligation around many of the atoms of twelve atoms at the corners of an approximately regular icosahedron. It is characteristic of the icosahedron that groups of four contiguous atoms occur only at corners of a tetrahedron; every triangle formed by three contiguous atoms in the icosahedron has a fourth atom lying approximately above its center. Accordingly, a structure involving icosahedral packing may be built up by placing atoms out from the centers of the triangular faces of an inner poly-

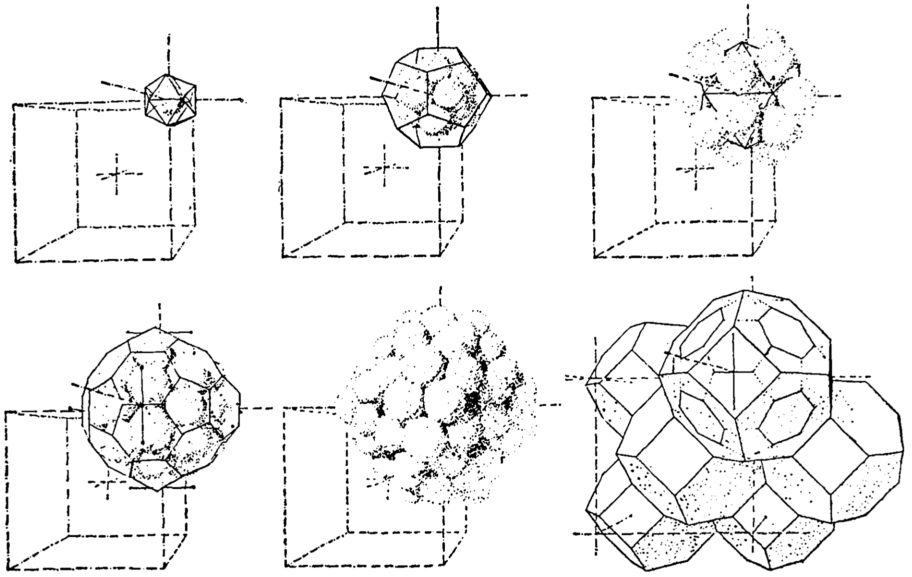

Fig. 1. The successive shells of atoms about the point (0,0,0) and the sharing of the outermost atoms between neighboring groups.

hedron. The metrical nature of the icosahedron is such that the distances from the atom at the center of an icosahedron to its twelve ligands is 5% smaller than the distances between these ligands; accordingly, the retention of icosahedral packing through successive ligation spheres requires a continued steady increase in average size of the atoms in these spheres. This increase in size can be achieved, for four spheres, by the use of the smaller atoms, zinc and aluminum, in the inner spheres, and the introduction of the larger magnesium atoms in the outer spheres.

The application of these arguments in the derivation of the structure for the phase $Mg_{32}(Zn, Al)_{49}$ proceeds as follows. In the first two drawings (upper left) of Fig. 1 there is shown a central atom with an icosahedral sphere of twelve atoms surrounding it. As shown in the next two drawings, twenty atoms may then be placed out from the centers of the twenty triangular faces of the icosahedron, forming a pentagonal dodecahedron, and twelve more out from the centers of the pentagonal faces of the dodecahedron. These thirty-two atoms constitute the third sphere of the aggregate; they lie at the corners of a rhombic triacontahedron. Sixty atoms, at the corners of a truncated icosahedron, may then be placed out from the centers of the sixty triangular half-rhombs of the triacontahedron, and by introducing twelve more atoms, as shown in the fifth and sixth drawings of Fig. 1, an outer sphere of seventy-two atoms lying on the faces of a cubooctahedron is obtained. Because of the property of cubooctahedra of packing together in a body-centered lattice, these complexes can be packed together in this way by sharing all of the seventy-two atoms of the outer shell with similar complexes. The resulting structure has seventy-two atoms, each of which serves as the outer shell of two adjacent complexes, and two inner groups of forty-five atoms each, about the positions 0, 0, 0 and $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$, giving a total of 162 atoms in the unit cube.

In this structure, 98 of the atoms have ligancy twelve (icosahedral coordination) and of the remaining 64 atoms 40 have ligancy sixteen, 12 have ligancy fifteen and 12 have ligancy fourteen. It is reasonable to assume the 98 icosahedral atoms to be either zinc or aluminum, and the others to be magnesium atoms. This assignment corresponds to the composition $Mg_{32}(Al, Zn)_{49}$, which is in reasonable agreement with $Mg_3Zn_3Al_2$.

Approximate atomic coordinates were obtained by assuming the effective metallic radius of magnesium to be about 1·60 Å and the radii of aluminum and zinc to be about 1·40 Å. The corresponding calculated structure factors were in fairly good agreement with those obtained from the observed intensities. The preliminary atomic coordinates are given in Table 1.

A set of improved atomic parameters was obtained from three successive Fourier projections on the *xy* plane, the first based on 34, the second on 56, and the third on 98 of the 126 observed *hk*0 reflections. From the heights of the peaks it was concluded that all or nearly all of the atoms in the position *B* are zinc atoms and that those in positions *C* and *F* are about 50% zinc atoms and 50% aluminum atoms. The peaks corresponding to the atoms in positions *A* were smaller than could be expected even for aluminum and were too small to appear on the third Fourier projection shown in Fig. 2.

Table 1. *Preliminary and final structural parameters*

Type of atom	Position		Positional parameters		Kind of atom
			Preliminary	Final	
A	2: (*a*)		—	—	(80%) Al
B	24: (*g*)	*y* =	0·11	0·0908	81% Zn
		z =	0·16	0·1501	19% Al
C	24: (*g*)	*y* =	0·19	0·1748	57% Zn
		z =	0·32	0·3007	43% Al
D	16: (*f*)	*x* =	0·19	0·1836	Mg
E	24: (*g*)	*y* =	0·32	0·2942	Mg
		z =	0·13	0·1194	
F	48: (*h*)	*x* =	0·16	0·1680	64% Zn
		y =	0·18	0·1860	36% Al
		z =	0·41	0·4031	
G	12: (*e*)	*x* =	0·40	0·4002	Mg
H	12: (*e*)	*x* =	0·20	0·1797	Mg

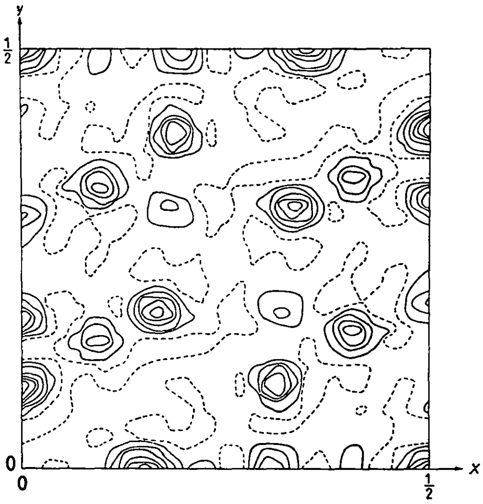

Fig. 2. The third Fourier projection on the *xy* plane. Contours at equal, arbitrary intervals.

The parameters were then further refined by four successive least-squares procedures, as described by Hughes (1941). Only *hk*0 data were used. The form factor for zinc was taken to be 2·4 times the average of the form factors for magnesium and aluminum. The values of the form factor for zinc used in making the average was corrected for the anomalous dispersion expected for copper *Kα* radiation. The customary Lorentz, polarization, temperature, and absorption factors were used. A preliminary combined scale, temperature, and absorption factor was evaluated graph-

Table 2. *Calculated and observed structure factors*

hkl	F_c	F_o	*hkl*	F_c	F_o	*hkl*	F_c	F_o	*hkl*	F_c	F_o
000	3143	—	910	−40	41	7,11,0	260	250	2,16,0	−96	120
110	185	125	390	110	78	11,7,0	−20	92	16,2,0	50	45
200	−60	22	930	67	62	3,13,0	38	52	8,14,0	53	56
220	−78	86	770	80	55	13,3,0	−39	87	14,8,0	85	37
130	−34	94	10,0,0	562	490	6,12,0	73	89	4,16,0	−37	33
310	181	180	680	−150	190	12,6,0	156	170	16,4,0	−11	36
400	−140	170	860	36	38	5,13,0	−46	43	7,15,0	−44	66
330	−98	115	2,10,0	−175	180	13,5,0	−69	65	15,7,0	−32	35
240	−104	120	10,2,0	−12	49	14,0,0	−66	43	12,12,0	91	93
420	74	75	590	−378	300	10,10,0	64	68	11,13,0	−33	54
150	−36	33	950	−352	300	2,14,0	21	55	13,11,0	111	135
510	−108	110	4,10,0	87	150	14,2,0	107	73	1,17,0	−1	19
440	−82	67	10,4,0	−199	210	9,11,0	−52	51	17,1,0	29	19
350	−682	550	11,1,0	−84	170	11,9,0	−124	140	6,16,0	97	45
530	−369	320	1,11,0	75	125	8,12,0	56	58	16,6,0	−105	125
600	800	590	880	54	49	12,8,0	−183	180	10,14,0	−29	27
260	28	27	3,11,0	−73	63	4,14,0	−27	70	14,10,0	18	75
620	24	37	11,3,0	−120	120	14,4,0	60	62	3,17,0	−97	93
170	43	61	790	83	70	7,13,0	47	47	17,3,0	−35	34
710	408	380	970	−117	97	13,7,0	22	48	9,15,0	−52	81
550	178	68	6,10,0	509	510	1,15,0	16	46	15,9,0	−53	48
460	−355	350	10,6,0	111	91	15,1,0	−10	46	5,17,0	70	28
640	128	135	12,0,0	416	360	6,14,0	−80	130	17,5,0	27	28
370	−156	165	5,11,0	133	69	14,6,0	−27	47	8,16,0	−28	20
730	8	95	11,5,0	−40	125	3,15,0	−156	180	16,8,0	1	20
800	−119	110	2,12,0	78	66	15,3,0	−44	47			
280	−51	48	12,2,0	−178	145	11,11,0	−44	83	435	539	*vs*
820	101	45	4,12,0	−53	84	10,12,0	157	155	666	−464	*vs*
660	22	46	12,4,0	−96	95	12,10,0	81	81	453	380	*vs*
570	−84	66	990	74	60	5,15,0	−123	140	1,12,1	−21	Abs.
750	20	46	8,10,0	−90	80	15,5,0	−49	53	341	5	Abs.
480	−1	57	10,8,0	−11	42	9,13,0	28	40	2,16,2	9	Abs.
840	94	85	1,13,0	24	46	13,9,0	51	63	233	24	Abs.
190	−33	63	13,1,0	203	200	16,0,0	71	68	455	18	Abs.
									11,5,6	3	Abs.

ically by plotting log (I_o/F_c^2) against $\sin^2 \theta$. The two parameters determining this factor were introduced in the least-squares refinement together with the twelve positional parameters and the four compositional parameters, these four parameters expressing the fraction of zinc atoms in the positions A, B, C, and F. The F_o values with weights proportional to F_o^{-2} were taken as observational quantities, and the normal equations were solved by application of the method described by Crout (1941). All the reflections were used in the final refinement; there were no accidentally absent reflections.

The reliability factor R was 0·276 after the first refinement and 0·211 after the fourth refinement. The parameters from the third and fourth refinements differed very little from one another. The final values are given in Table 1. As large systematic errors were introduced in the refinement process by the unavoidable use of very poor atomic form factors, the probable errors in the parameters as obtained in the refinement were considered to be of questionable significance. For this reason they are not given in the table. The average error was, however, estimated to be 0·001 for the positional parameters and 5% for the compositional parameters. The scattering power of the two atoms of type A was given by the least-squares refinement as only 0·8 times that of aluminum (the fraction zinc in positions A was −14%). The significance of this result is discussed below. Atoms of type B are indicated to be about 80% zinc and 20% aluminum, and those of types C and D about 60% zinc and 40% aluminum.

The observed and calculated values of F for prism planes are given in Table 2.

Discussion of the structure

In this structure there are two predominant coordination polyhedra: all of the 98 zinc and aluminum atoms in the unit cell have icosahedral coordination, and 40 of the 64 magnesium atoms have a coordination polyhedron with sixteen corners and twenty-eight triangular faces, which was first observed for the magnesium atoms in the Friauf phase $MgCu_2$ (Friauf, 1927). Twelve of the remaining twenty-four magnesium atoms (H) have ligancy 15, the coordination polyhedron being bounded by twenty-six triangular faces, and the other twelve (G) have ligancy fourteen, the polyhedron being bounded by twenty-four triangular faces. All four of the polyhedra are shown in Fig. 3 in the sequence in which they were discussed above.

Interatomic distances are given in Table 3. There are some very short (Zn, Al)–(Zn, Al) distances in the structure: A–B = 2·484 and B–C = 2·442 Å. These

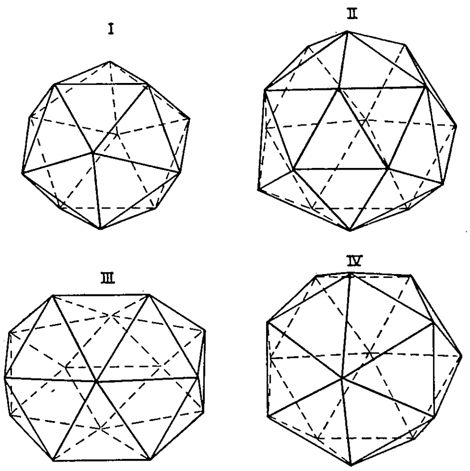

Fig. 3. The four different coordination polyhedra in the $Mg_{32}(Al, Zn)_{49}$ structure.

Table 3. *Interatomic distances*

(All values in Ångström units)

A–B	12	2·484
B–A	1	2·484
B–B	4	2·622
B–B	1	2·571
B–C	1	2·442
B–D	2	3·274
B–E	1	2·908
B–E	2	2·945
	12	
C–B	1	2·442
C–D	2	3·326
C–E	1	3·074
C–E	2	2·992
C–F	2	2·791
C–F	2	2·624
C–G	1	3·016
C–H	1	3·494
	12	
D–B	3	3·274
D–C	3	3·326
D–D	1	3·257
D–E	3	3·168
D–F	3	3·116
D–F	3	3·055
	16	
E–B	1	2·908
E–B	2	2·945
E–C	1	3·074
E–C	2	2·992
E–D	2	3·168
E–E	1	3·381
E–F	2	3·132
E–F	2	3·123
E–G	2	3·652
E–H	1	2·927
	16	
F–C	1	2·791
F–C	1	2·624
F–D	1	3·116
F–D	1	3·055
F–E	1	3·132
F–E	1	3·123
F–F	2	2·621
F–F	1	2·747
F–G	1	3·005
F–H	1	3·344
F–H	1	2·974
	12	
G–C	2	3·016
G–E	4	3·652
G–F	4	3·005
G–G	1	2·832
G–H	2	2·911
G–H	1	3·122
	14	
H–C	2	3·494
H–E	2	2·927
H–F	4	3·344
H–F	4	2·974
H–G	2	2·911
H–G	1	3·122
	15	

short distances appear less remarkable in view of the fact that some evidence was obtained for only partial occupancy of the positions *A*. Both the last Fourier projection and the last least-squares refinement provided such evidence. In case of partial occupancy the *A–B* distance can be expected to be shortened considerably. If the assumption of partial occupancy is not correct it is likely that these bonds are under compressional strain, and that the bond numbers obtained by application of the equation $R_n = R_1 - 0{\cdot}300 \log_{10} n$ are larger than the true values. Moreover, it is likely that some transfer of valence electrons from the zinc atoms to atoms of magnesium and aluminum has taken place (Pauling, 1950). Values of effective valences of seven of the eight crystallographically different kinds of atoms have been calculated by use of assumed radii for magnesium and zinc/aluminum atoms. The value 1·214 Å for the single bond radius may be used for the zinc/aluminum atoms *B*, *C*, and *F*, and the value 1·335 Å for magnesium, which may be assumed to have accepted one half an electron, increasing its valency to 2·5. The values of the valences obtained in this way are 4·87 for *B*, 2·17 for *C*, and 2·80 for *F* (these being zinc/aluminum atoms); and 1·95 for *D*, 2·44 for *E*, 2·35 for *G*, and 2·56 for *H* (these being magnesium atoms). Because of uncertainties in the argument, these values of the valences of the different kinds of atoms are not very reliable. The value of the effective valence of the atoms *A* was not calculated because of the definite possibility of partial occupancy. In case of partial occupancy a correction of the valence of atoms *B* as calculated above should be made.

The nature of the structure found for this phase, with strong indication that there are thirty-two magnesium atoms per lattice point, suggests that the quaternary phase should be assigned the general formula $Mg_{32}(Al, Zn, Cu)_{49}$.

Attempts to relate the stability of this phase to the filling of a Brillouin zone were not successful: no well-defined zone could be found.

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Dispositif Permettant l'Étude aux Rayons X par Réflexion de la Diffusion au Voisinage des Nœuds du Réseau Reciproque

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(*Reçu le* 15 *octobre* 1956)

A technique is described for studying the diffuse scattering in the neighbourhood of the Bragg reflexions from alloy crystals which undergo structural hardening. It employs strictly monochromatic radiation focused by reflexion.

Description de la méthode

L'étude de la répartition de l'intensité diffusée au voisinage immédiat des taches de Bragg, est souvent difficile pour les alliages à durcissement structural, par suite de l'étalement géométrique de la tache elle-même, étalement qui réduit le pouvoir séparateur. On peut utiliser un microfaisceau ou un microcristal, mais les temps de pose sont longs, parce que l'intensité diffusée est faible et que le rayonnement n'est pas rigoureusement monochromatique.

Nous avons employé la méthode suivante pour déterminer la forme des nœuds satellites qui apparaissent lors du vieillissement d'alliages à base de nickel. La méthode est dérivée du montage à deux monochromateurs croisés de Shenfil, Danielson & DuMond (1952) reprise par Rose & Barraud (1955).

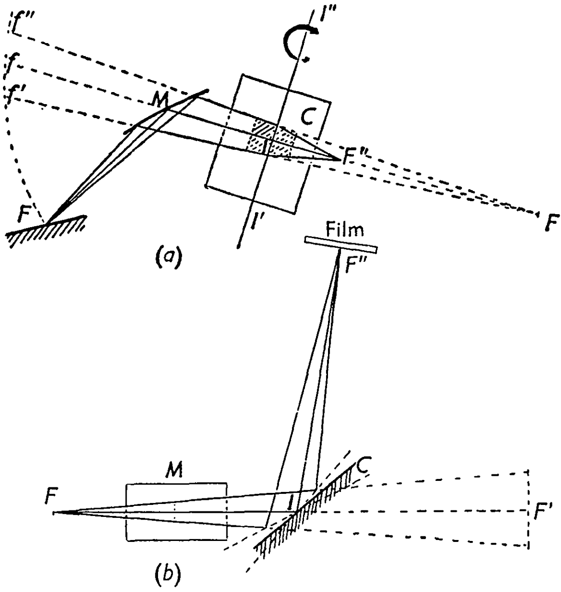

Fig. 1. Schémas de principe du montage.

Ici nous avons utilisé un seul monochromateur et remplacé le deuxième par le ou les cristaux à étudier (Fig. 1(*a*) et (*b*)).

Sur le dessin (Fig. 1(*a*)), l'axe de courbure du monochromateur *M* est vertical.

Les rayons X issus du foyer ponctuel *F* du tube sont réfléchis par le monochromateur dissymétrique *M*, et viennent se concentrer en *F'* en l'absence du cristal *C*, suivant une focale presque rectiligne. Le monochromateur peut réfléchir le rayonnement avec une ouverture verticale de 2° environ grâce à la largeur spectrale de $\lambda K\alpha_1$ utilisée et des imperfections du cristal de quartz. C'est surtout la première cause qui intervient.

Les rayons qui passent en *F'* semblent provenir d'un arc de cercle *f'ff''*.

Le cristal à étudier *C* est une plaquette; il a son plan réflecteur parallèle à la face, elle-même contenant l'axe *I'I''* horizontal et perpendiculaire à *fF'*. Le point *I* de l'axe *I'I''* est situé à mi-distance de *fF'* et au centre du cristal *C*. Lorsque *C* tourne autour de l'axe *I'I''* les rayons issus de *f* sont réfléchis et viennent passer successivement en un point *F''* tel que $fI = IF''$. Pour les rayons issus de *f'f''* il y a focalisation approximative au point *F''*.

Les causes d'aberrations sont les suivantes:

(*a*) La hauteur du foyer *F*.
(*b*) La dissymétrie des distances focales du monochromateur *M*, d'où il résulte une différence des distances *f'F'*, *fF'* et *f''F'* donc un élargissement radial de la tache focale.