The Structure of α (Al–Cu–Fe)

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The structure of α(Al–Cu–Fe), isomorphous with $MnAl_6$, has been refined using two-dimensional projections. The centrosymmetric space group *Ccmm* was chosen, but the ellipticity of a number of the projected atomic peaks was considered to be too large to be the result of anisotropic thermal motion. The ellipticities are successfully explained in terms of a symmetry debasement to the non-centrosymmetric space group $Ccm2_1$, although it has not been possible to decide between alternative directions for the small atomic shifts which give rise to this symmetry debasement.

1. Introduction

A detailed study of the aluminium-rich corner of the (Al–Cu–Fe) phase diagram by Phillips (1953–54) has confirmed the earlier work of Phragmén (1950), and established the primary field for the α-phase as shown in Fig. 1. Phragmén assigned a formula $(FeCu)(CuAl)_6$ to the α-phase, and because the unit-cell dimensions and symmetry were very similar to those of $MnAl_6$ (Hofmann, 1938) he regarded it as a copper-stabilized $FeAl_6$, a phase which does not occur in the binary phase diagram. The composition of Phragmén's crystals was given as Al 70%, Cu 8%, Fe 22% by weight. Attempts to prepare a single-phase ingot by Phillips were unsuccessful.
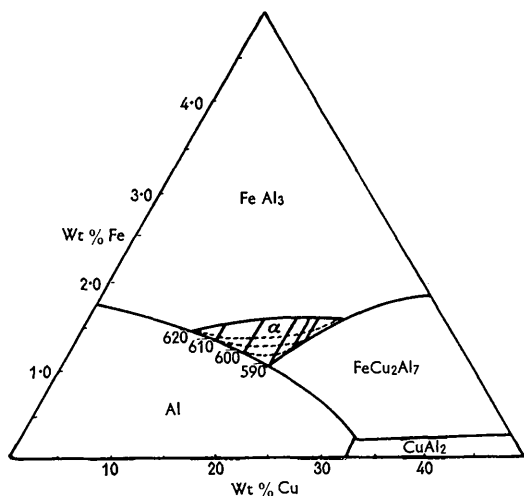

Fig. 1. Aluminium-rich corner of the (Al–Cu–Fe) phase diagram.

The structure of $MnAl_6$ is known (Nicol, 1953), and a refinement of the structure of $(FeCu)(CuAl)_6$ was

undertaken so that the effect on the structure of the change in transition metal could be studied.

2. Material

A few crystals (*H*) of the α-phase were kindly supplied by Dr A. Harding, of the Aluminium Research Laboratories, Banbury. They were extracted, using a 1–2% HCl solution, from a melt of composition 80·7% Al, 18·0% Cu, 1·3% Fe, by weight, which had been held at 590–618 °C. for some hours and then quenched. All materials were super-pure. The crystals possess the same habit as those of $MnAl_6$-prismatic needles bounded by {110} faces.

After the X-ray measurements had been made, two further samples became available; Dr P. Spiegelberg sent us some of Phragmén's original specimens (*P*) from the Metallografiska Institutet, Stockholm, and Mrs J. Y. Halnan, of the Aluminium Research Laboratories, gave us some crystals (*A*) which had been selected as being without $FeAl_3$ cores.

3. Unit cell, density and composition

The cell dimensions (*H* crystals), measured using a Farquhar–Lipson (1946) camera, are:

$$a = 6{\cdot}4343 \pm 0{\cdot}0001, \quad b = 7{\cdot}4604 \pm 0{\cdot}001 ,$$
$$c = 8{\cdot}7769 \pm 0{\cdot}001 \text{ Å} .$$

The density, measured by a flotation method, is $3{\cdot}62 \pm 0{\cdot}01$ g.cm.$^{-3}$. The same method applied to some *P* crystals gave a value of $3{\cdot}52 \pm 0{\cdot}01$ g.cm.$^{-3}$, whereas the density of the *P* crystals calculated for 28 atoms per unit cell (see below) in $3{\cdot}53$ g.cm.$^{-3}$.

Insufficient material was available for either chemical or ultra-violet spectroscopic analysis of the *H* crystals. Two attempts to obtain an accurate value for the Cu:Fe ratio in these crystals using X-ray fluorescence analysis techniques failed. When finally an accurate method had been devised by Dr P. Jane Brown (1960), the only remaining *H* specimens were cored by $FeAl_3$. The Cu:Fe ratio was, however,

Table 1. *Unit cell dimensions and compositions of the α-phase specimens*

Specimen	a (Å)	b (Å)	c (Å)	Cu:Fe ratio wt.%
P*	6·441	7·464	8·786	35·8 ± 0·6
A	6·4359 ± 0·0003		8·7774 ± 0·0003	31·0 ± 0·6
H	6·4343 ± 0·0001	7·4604 ± 0·001	8·7769 ± 0·001	30·0 ± 1·8

* Taken from Phragmén's (1950) paper in which no limits of error are quoted.

determined by this method for the P and A materials, and the probable Cu:Fe ratio in the H crystals estimated by comparing the cell dimensions of all three types. The a and c dimensions showed the greatest variation between the P and the H crystals, so these were measured for an A specimen using the Farquhar–Lipson camera; the results are summarized in Table 1. The cell dimensions of the P crystals are those quoted by Phragmén (1950) and the Cu:Fe ratio compares satisfactorily with the value 36% obtained from his chemical analysis of the composition. The H cell dimensions are near to those of the A crystals and indicate a Cu:Fe ratio of 30·0 ± 1·8% by wt. This ratio, together with the density and a unit-cell volume of 421·3 Å³, gives a value of 4·24 ± 0·17 as the number of iron atoms in the unit cell, assuming that all the 28 atomic sites are fully occupied. This value is probably not significantly different from 4·0 and, as it is unlikely that any iron atoms would go into aluminium sites, this value has been adopted, giving a unit-cell content of $Fe_{4.0}Cu_{1.05}Al_{22.95}$.

4. X-ray intensity data

Reflexions from the [010] and [001] zones of an H crystal were collected on zero-layer Weissenberg photographs from a crystal of approximately cubic shape and side 0·11 mm.; filtered Mo $K\alpha$ radiation and packs of three films were used. The intensities were measured by visual comparison with an intensity scale made with the same crystal. Corrections for the Lorentz and polarization factors were made, but none for absorption, except for the special purpose described in Section 6.

Laue and oscillation photographs showed the space group to be either Ccmm (centrosymmetric), Ccm2₁ or Cc2m (non-centrosymmetric).*

5. Approximate structure

The intensities of the reflexions were similar to those obtained from $MnAl_6$ (Nicol 1953) and refinement was started using the centro-symmetric space group Ccmm (since Wilson statistical tests [Wilson 1949, 1950] indicated centrosymmetry) and the $MnAl_6$ atomic parameters, with Fe taking the place of Mn (since the proportion of Cu in the alloy was small). Fig. 2(a) shows the asymmetric unit of the structure in the

* These space-groups are not in the orientation adopted by the new *International Tables* because the axes have been chosen to correspond to those for $MnAl_6$ (Nicol, 1953).
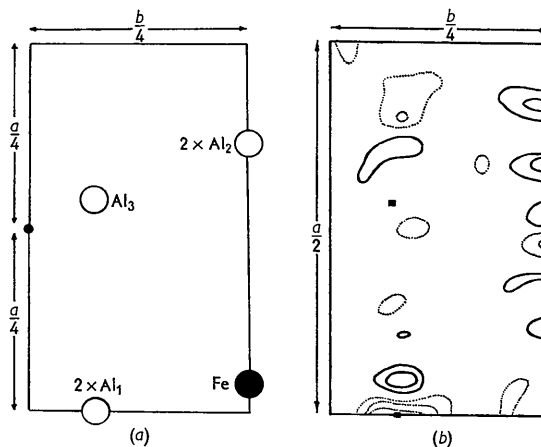

Fig. 2. α(Al–Cu–Fe) [001] projection. (a) Asymmetric unit of the centrosymmetric structure ● indicates the centre of symmetry in this projection. (b) Corresponding $(F_o - F_c)$ Fourier synthesis at $R = 0.17$. Contours have been drawn at one fifth the interval used for the F_o map in Fig. 4(a). Negative contours are shown as broken lines, the zero contour being omitted.

[001] zone and Fig. 2(b) the $(F_o - F_c)$ map for this projection at an R factor of 0·17. The most significant features of this $(F_o - F_c)$ map are the peaks on either side of the Al_1, Al_2 atomic positions in the x direction. The same effects appeared on the [010] $(F_o - F_c)$ map and, in addition, peaks existed on either side of the Al_3 position in the z direction. In this structure, these peaks may be interpreted *either* in terms of a large anisotropic temperature factor for the aluminium atoms, *or* as an indication that the structure has lower symmetry than that required by the space group Ccmm.

6. Refinement of the structure

The possibility of a marked anosotropy in the thermal vibrations of the aluminium atoms was considered unlikely. No indication of such an anisotropy had been seen on the last $(F_o - F_c)$ projections of a number of similar intermetallic phases studied in this Laboratory, (see for example Black (1954), Robinson (1951)), and the mean temperature factors determined for these compounds were very low, being of the order of $B = 0.5 \times 10^{-16}$ cm.². The mean temperature factor for the α-phase, as determined from a plot of the logarithm of the scaling factor F_o/F_c, against $\sin^2 \theta/\lambda^2$ for the high angle reflexions, was $B = 0.39 \times 10^{-16}$ cm.². In this evaluation, an absorption correction was applied to the observed intensities by assuming that the

specimen approximated to a cylinder and using the coefficients given by Bradley (1935).

The atomic positions at this stage were:

$$(0, 0, 0; \tfrac{1}{2}, \tfrac{1}{2}, 0)+$$

4 Fe at $(x, 0, \tfrac{1}{4})$; $(\bar{x}, 0, \tfrac{3}{4})$;

8 Al$_1$ at $(0, y, 0)$; $(0, \bar{y}, 0)$; $(0, y, \tfrac{1}{2})$; $(0, \bar{y}, \tfrac{1}{2})$;

8 Al$_2$ at $(x, 0, z)$; $(x, 0, \tfrac{1}{2}-z)$; $(\bar{x}, 0, \tfrac{1}{2}+z)$; $(\bar{x}, 0, \bar{z})$;

8 Al$_3$ at $(x, y, \tfrac{1}{4})$; $(x, \bar{y}, \tfrac{1}{4})$; $(\bar{x}, y, \tfrac{3}{4})$; $(\bar{x}, \bar{y}, \tfrac{3}{4})$.

If the (F_o-F_c) maps are to be interpreted in terms of atomic shifts, the space group must be changed to $Ccm2_1$. The removal of the mirror plane perpendicular to c doubles the asymmetric unit in the z direction, and the atomic positions are then grouped as follows:

$$(0, 0, 0; \tfrac{1}{2}, \tfrac{1}{2}, 0)+$$

4 Fe at $(x_0, 0, z_0)$; $(\bar{x}_0, 0, \bar{z}_0)$;

8 Al$_1$ at (x_1, y_1, z_1); $(\bar{x}_1, y_1, \tfrac{1}{2}+z_1)$; $(x_1, \bar{y}_1, z_1)$;
$(\bar{x}_1, \bar{y}_1, \tfrac{1}{2}+z_1)$;

8 Al$_3$ at (x_3, y_3, z_3); $(\bar{x}_3, y_3, \tfrac{1}{2}+z_3)$; $(x_3, \bar{y}_3, z_3)$;
$(\bar{x}_3, \bar{y}_3, \tfrac{1}{2}+z_3)$;

$\left.\begin{array}{l} 4\ \text{Al}_2 \\ 4\ \text{Al}_4 \end{array}\right\}$ previously 8 Al$_2$ $\left\{\begin{array}{l} \text{at } (x_2, 0, z_2);\ (\bar{x}_2, 0, \bar{z}_2); \\ \text{at } (x_4, 0, z_4);\ (\bar{x}_4, 0, \bar{z}_4); \end{array}\right.$

with $z_0, z_3 \approx \tfrac{1}{4}$ and $x_1, z_1 \approx 0$.

These co-ordinates allow movements to be made to the aluminium atoms which result in a levelling of the (F_o-F_c) synthesis. The origin of co-ordinates was chosen so that $z_1=0$. The steps in the refinement are outlined below.

(a) [001] zone.

This zone is still centrosymmetric in projection. The contents of the asymmetric unit are shown in Fig.3(a). The two Al$_1$ atoms are related by the c glide plane perpendicular to a, and may only have equal and opposite displacements, in the x direction, from their original superposed positions. The independent Al$_2$, Al$_4$ atoms were moved in opposite directions, again in the x direction about the mean position previously occupied by Al$_2$ (Fig. 2(a)), though it was impossible to say which of the two z-coordinates of the previously related pair corresponded to a particular x-coordinate. The final (F_o-F_c) map for the projection is shown in Fig. 3(b): the R factor was then 0·10.

(b) [010] zone

This projection was centrosymmetric in the approximate structure, and the departures from this symmetry are small. The ambiguity in assigning shifts to the Al$_2$ and Al$_4$ atoms affects this projection. There are two possible $x-z$ combinations and improvement in the cosine contribution to F_{h0l} results if the small atomic shifts are carried out in either of the two possible directions: the sine terms make only a small contribution to the magnitude and change in phase of the F_{h0l} terms. Consequently, it is difficult to choose between each pair of directions, either from the point of view of the R factor, or of the (F_o-F_c) synthesis.
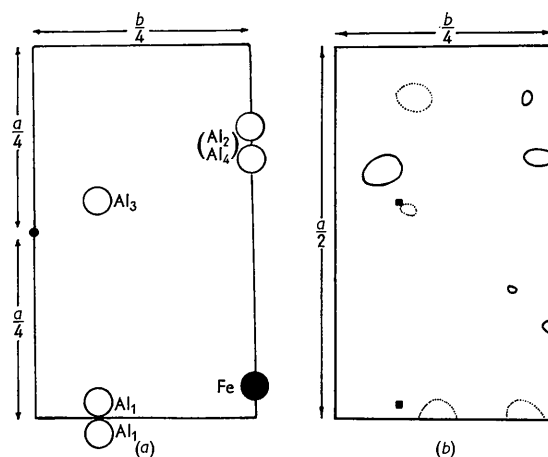

Fig. 3. α(Al–Cu–Fe) [001] projection. (a) Asymmetric unit of the non-centrosymmetric structures. (b) Corresponding (F_o-F_c) Fourier synthesis: contours as for Fig. 2(b).

The movement of the Al$_1$ atom in the x direction was taken as the reference one and the Al$_3$, Al$_2$ and Al$_4$ atoms were moved relative to this displacement. During the refinement it was found that no alteration was required in z_0, but that a shift in z_3 was necessary. The two Al$_3$ atoms are superposed by the b-axis mirror plane and they appeared in negative regions of the (F_o-F_c) map with positive areas on either side of them in the z-direction [cf. Al$_1$ atoms in Fig. 2(b)]. An ambiguity arises again as the (F_o-F_c) map is improved when the parameter z_3 is either increased or decreased.
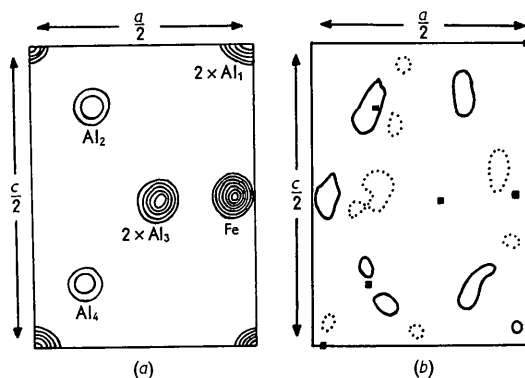

Fig. 4. α(Al–Cu–Fe) [010] projection. (a) F_o Fourier synthesis map of the asymmetric unit of structure B. Contours are at equal arbitrary intervals. (b) Corresponding (F_o-F_c) Fourier synthesis map: contours as for Fig. 2(b).

Table 2. *Key to the atomic shifts adopted in the structures A, B, C and D, together with the final R-factors.*

Structure	Atom Al$_3$: z_3	Atom Al$_2$: x_2	Atom Al$_4$: x_4	R-Factor
A	< 0·2500	> mean	< mean	0·12
B	< 0·2500	< mean	> mean	0·11
C	> 0·2500	> mean	< mean	0·11
D	> 0·2500	< mean	> mean	0·12

Table 3. *Atomic parameters in* α(Al–Cu–Fe) *and their standard deviations*

Structure parameter	Centro-symmetric	Standard deviation	A	B	C	D	Standard deviation
x_0	0·4612	0·0002	0·4612	0·4612	0·4612	0·4612	0·0003
z_0	$\frac{1}{4}$	—	0·2500	0·2500	0·2500	0·2500	0·0005
x_1	0	—	0·0171	0·0171	0·0171	0·0171	0·0016
y_1	0·3255	0·0002	0·3255	0·3255	0·3255	0·3255	0·0003
x_3	0·2872	0·0005	0·2872	0·2872	0·2872	0·2872	0·0009
y_3	0·3182	0·0003	0·3182	0·3182	0·3182	0·3182	0·0006
z_3	$\frac{1}{4}$	—	0·2410	0·2610	0·2415	0·2580	0·0005
x_2	0·1300	0·0011	0·1450	0·1450	0·1210	0·1210	0·0022
z_2	0·1050	0·0006	0·1051	0·1050	0·1050	0·1060	0·0012
x_4	$= x_2$	0·0011	0·1210	0·1210	0·1450	0·1450	0·0022
z_4	$= (\frac{1}{4} - z_2)$	0·0006	0·3940	0·3970	0·3970	0·3980	0·0012

The ambiguities mentioned in the two preceding paragraphs combine to give four possible combinations of directions of shifts. These are designated A, B, C and D, and a key to them is given in Table 2. Once a set of shift directions had been chosen, the refinement was continued to the best answer and, in some cases, the amounts of shift differ slightly. All four final $(F_o - F_c)$ maps had no further significant slopes, and that for structure B is shown in Fig. 4(b) together with the corresponding F_0 synthesis in Fig. 4(a).

Table 3 gives the atomic parameters for the different structures, together with their standard deviations, which have been assessed by the method suggested by Lipson & Cochran (1953). A complete list of F_o and F_c values is available elsewhere (Forsyth 1959).

7. Discussion

The structure is basically similar to that of MnAl$_6$, fully described by Nicol (1953). Further work is being carried out on MnAl$_6$, and it is interesting to note that effects are also observed in this structure which, though smaller in magnitude, are similar to those interpreted in terms of a slight departure from centro-symmetry in α(Al–Cu–Fe). A detailed discussion of the relationships between the two structures is reserved until the refinement of MnAl$_6$ is completed; in the following sections reference is to the published MnAl$_6$ structure.

Attention may be directed to two points in relation to the refinement procedure described in Section 6. In the first place, no low-temperature study has been made which could confirm the absence of anisotropic thermal vibrations associated with the aluminium atoms, but the root-mean-square displacement associated with the observed mean temperature factor is 0·050 Å; this would have to be increased by a factor of about four, in the directions of greatest vibration, for effects to be obtained which are equivalent to those produced by altering the atomic positions. Secondly, when the symmetry conditions were relaxed, it was not possible, using photographically-recorded X-ray diffraction data, to decide between the alternatives presented in the last stages of refinement. The various

combinations of ambiguous shifts do not give rise to any changes in $F_c(h0l)$, even for specially selected reflections, which are large enough to enable a choice between the structures to be made. This is primarily due to the small values of the sine components of the structure factors. The shift in one pair (Al$_{2,4}$) of atoms is approximately parallel to the a-axis so that a [100] projection could not help resolve this ambiguity. The remaining ambiguity, involving the z-coordinate of Al$_3$, would affect a [100] projection in exactly the same way as the [010] projection, for in both cases the atom is clearly resolved. It therefore seems unlikely that any further clarification could be obtained by refining the third projection using eye-estimated intensities. Three-dimensional data would only help in so far as they gave more accurate syntheses.
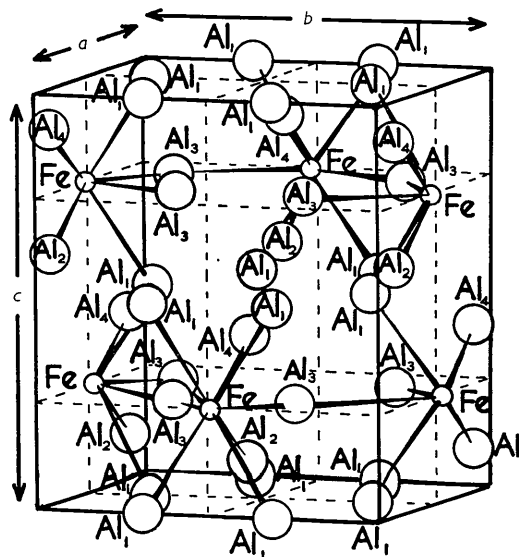

Fig. 5. Atomic arrangement in α(Al–Cu–Fe).

Fig. 5 shows the approximate distribution of the atoms in the unit cell and corresponds to a diagram in the paper by Nicol (1953): Table 4 gives a list of the interatomic distances together with their estimated errors. The environment of the iron atoms is not significantly different whichever structure A, B,

Table 4. *Interatomic distances in* α(Al–Cu–Fe) *and their standard deviations*

Atom	Bonded to	Centrosymmetric structure No. of bonds	Length (Å)	Standard deviation	Non-centrosymmetric structure No. of bonds	Length (Å) A	B	C	D	Standard deviation
Fe	Al₁	4	2·571	0·002	2	2·576	2·576	2·576	2·576	0·003
	Al₁	—	—	—	2	2·555	2·555	2·555	2·555	0·003
	Al₂	2	2·478	0·008	1	2·400	2·400	2·532	2·527	0·015
	Al₃	2	2·623	0·004	2	2·626	2·626	2·626	2·625	0·007
	Al₃	2	2·500	0·004	2	2·499	2·500	2·499	2·499	0·007
	Al₄	—	—	—	1	2·527	2·541	2·409	2·414	0·015
Al₁	Fe	2	2·571	0·002	1	2·555	2·555	2·555	2·555	0·003
	Fe	—	—	—	1	2·576	2·576	2·576	2·576	0·003
	Al₁	1	2·603	0·003	1	2·603	2·603	2·603	2·603	0·004
	Al₂	2	2·872	0·006	1	2·877	2·877	> 3	> 3	0·013
	Al₂	2	2·715	0·003	1	2·724	2·724	2·682	2·685	0·004
	Al₃	2	2·795	0·003	1	2·795	2·930	2·794	2·909	0·010
	Al₃	—	—	—	1	2·811	2·671	2·807	2·692	0·010
	Al₃	2	2·872	0·003	1	2·738	2·876	2·741	2·855	0·009
	Al₃	—	—	—	1	> 3	2·870	2·997	2·889	0·009
	Al₄	—	—	—	1	2·825	2·817	2·690	2·690	0·013
	Al₄	—	—	—	1	2·748	2·739	2·793	2·793	0·004
Al₃	Fe	1	2·500	0·004	1	2·499	2·500	2·499	2·499	0·007
	Fe	1	2·623	0·004	1	2·626	2·626	2·626	2·625	0·007
	Al₁	2	2·795	0·003	1	2·811	2·671	2·807	2·692	0·010
	Al₁	—	—	—	1	2·795	2·930	2·798	2·909	0·010
	Al₁	2	2·868	0·003	1	> 3	2·870	2·997	2·889	0·009
	Al₁	—	—	—	1	2·738	2·876	2·741	2·855	0·009
	Al₂	2	2·877	0·006	1	2·810	2·889	2·866	2·925	0·013
	Al₄	—	—	—	1	2·929	2·864	2·887	2·825	0·013
	Al₂	2	2·886	0·006	1	2·926	> 3	2·808	2·869	0·013
	Al₄	—	—	—	1	2·873	2·806	> 3	2·937	0·013
	Al₃	1	2·712	0·005	1	2·712	2·712	2·712	2·712	0·012
Al₂	Fe	1	2·478	0·008	1	2·400	2·400	2·532	2·527	0·015
	Al₁	2	2·715	0·003	2	2·724	2·724	2·682	2·685	0·004
	Al₁	2	2·872	0·006	2	2·877	2·877	> 3	> 3	0·013
	Al₃	2	2·877	0·006	2	2·810	2·889	2·866	2·935	0·013
	Al₃	2	2·886	0·006	2	2·926	> 3	2·808	2·869	0·013
	Al₄(Al₂)	1	2·545	0·011	1	2·541	2·567	2·567	2·567	0·015
	Al₄(Al₂)	1	2·489	0·014	1	2·521	2·502	2·502	2·509	0·018
Al₄	Fe			.	1	2·527	2·541	2·409	2·414	0·015
	Al₁				2	2·748	2·739	2·793	2·790	0·004
	Al₁				2	2·825	2·817	2·690	2·687	0·013
	Al₃				2	2·929	2·864	2·887	2·825	0·013
	Al₃				2	2·873	2·806	> 3	2·941	0·013
	Al₂				1	2·541	2·567	2·567	2·567	0·015
	Al₂				1	2·521	2·502	2·502	2·502	0·018

C or D is chosen, and in each structure the Al₂ atom has only one transition metal (T.M.) neighbour, as in MnAl₆. The T.M.–Al₂ bond is significantly longer in the centrosymmetrical structure of the phase than in MnAl₆ (2·48 Å compared with 2·43₅ Å), but in the structures, A, B, C and D the Al₂ sites are changed into two fourfold Al₂, Al₄ sites: in each structure one of these fourfold sites has a short T.M.–Al distance of 2·40–2·41 Å, while the other has a T.M.–Al bond length of 2·53–2·54 Å. The numbers of aluminium-atom neighbours in the four structures are given in Table 5, the upper limit of distance for a neighbour being taken as 2·9 Å. It can be seen that the structures A, B, C and D have lower co-ordination numbers than the centrosymmetric structures in all but one case (the Al₄ atom in structure B).

Table 5. *Numbers of neighbours to aluminium atoms in* α(Al–Cu–Fe)

Atom	Number of neighbours Structure Centro-symmetric	A	B	C	D
Al₁	11	10	10	9	9
Al₃	11	8	9	9	8
Al₂	11	9*	9*	9	7
Al₄	11	9	11	9*	9*

* This number includes the short Al–T.M. bond.

The mean Fe–Al–Fe distances for the Al₁ and Al₃ atoms are slightly shorter than the corresponding distances in MnAl₆ but there is no change in the angle

subtended at the aluminium atom, which is in accordance with a suggestion made by Brown (1957)*.

Phillips (1953–54) suggested that the composition of the α-phase should be represented by $Fe(Cu_{0.04}Al_{0.96})_6$ and reasoned that the copper atoms were most likely to enter the Al_2 atomic sites. The measurements of composition reported above indicate strongly that the copper only replaces aluminium, though to a slightly greater extent than expected by Phillips; the corresponding formula is $Fe(Cu_{0.044}Al_{0.956})_6$. The Al_2 sites would appear to be the most favourable positions for copper atoms in view of the short bond length to the T.M. neighbour. In the non-centrosymmetric structures, the site with the shorter T.M. bond would be preferred, but complete ordering of the copper atoms on one rather than the other of the $Al_{2,4}$ sites might not take place with ordinary annealing times.

If all the copper atoms were ordered on one 8-fold aluminium site, a difference of 16% between the height of these 'Al' peaks in the electron density maps and those of the Al_1 and Al_3 atoms would be expected. The Al_2 site is the only one which is situated on a positive peak in the final $(F_o - F_c)$ maps, but the effect shown is much less than 16% and is probably not significant.

No attempt has been made to detect electron transfer in this structure [Black (1955) and Taylor (1954)], and the uncertainty about the composition makes this alloy unsuitable as a subject for further investigation using a counter diffractometer.

We are grateful to Professor N. F. Mott and Dr

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* Brown (1957) has noted that the occurrence of short T.M.–Al bonds in this type of compound is nearly always associated with the Al atom being joined to two T.M. atoms with a T.M.–Al–T.M. inter-bond angle approaching 180°. The bonds increase in length with decreasing inter-bond angle and the angle subtended at an Al atom by two T.M. atoms at a given distance is greater for manganese than for cobalt. Brown has suggested that iron would be intermediate between manganese and cobalt in this respect.

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Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible. Publication will be quicker if the contributions are without illustrations.

The unit cell and space group of MgGeO₃. By W. LINDEMANN, *Mineralogisches Institut der Universität Erlangen, Germany*

Synthetic $MgGeO_3$ used for this determination was prepared by heating a stoichiometric oxide mixture at 1220 °C. for 2 days. Several X-ray photographs have been taken using Cu $K\alpha$ and Fe $K\alpha$ radiation. Rotation and Weissenberg photographs have shown the unit cell to be orthorhombic with dimensions:

$$a = 18.649 \pm 0.007, \quad b = 8.902 \pm 0.005, \quad c = 5.332 \pm 0.005 \text{ Å}.$$

The systematic absences observed are those of the space group D_{2h}^{15}–$Pbca$. The measured crystal density is 4.31 g.cm.⁻³, giving 16 formula units per unit cell. The calculated density is 4.320 g.cm.⁻³.

No further work on this compound is contemplated.