

# STRUCTURE REPORTS

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UTRECHT

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## SYMBOLS

The letters  $a, b, c; \alpha, \beta, \gamma$  are used consistently for the edges and angles of the unit cell. Other letters used consistently are as follow.

$U$	Volume of unit cell
$D_m$	Measured density or specific gravity
$D_x$	Density calculated from cell volume and contents
$Z$	Number of times the formula quoted is repeated in the unit cell (Number of atoms per unit cell in alloys of simple structure)
$x, y, z$	Atomic coordinates as fractions of cell edge (Occasionally $u, v, w$ or other letters are used)
$X, Y, Z$	Atomic coordinates in Ångström units
$X', Y, Z'$	Atomic coordinates in Ångström units, referred to orthogonal axes (Used only in the Organic Section)
F.W.	Formula weight
$A, B, C$	Types of layer in layer structures
$M, A, B$	Variable metal atom(s) in a sequence of related structures
$X, H$	Variable non-metals, usually halogen, in a sequence of related structures
$R$	Variable organic radical
$s, m, w, v, b$	Strong, medium, weak, very, broad

## LIMITS OF ERROR

Errors are quoted in units in the last place. Thus  $4.8754 \pm 3$  means  $4.8754 \pm 0.0003$ ,  $4.87 \pm 3$  means  $4.87 \pm 0.03$ , and  $4.875 \pm 15$  means  $4.875 \pm 0.015$ . Occasionally a very doubtful last digit has been placed in parentheses.

## TRANSLITERATION OF RUSSIAN

а	а	и	і	р	г	ш	š
б	б	й	ј	с	с	щ	šč
в	в	к	к	т	т	ы	у
г	г	л	л	у	у	ъ	”
д	д	м	м	ф	ф	ь	’
е	е	н	п	х	kh	э	ě
ж	ž	о	о	ц	с	ю	ju
з	z	п	р	ч	č	я	ja

## INTRODUCTION

*Structure Reports* are not intended to be abstracts in the ordinary sense. Ideally they extract only the material of structural interest in the paper reported, and attempt to do this so completely that no further structural information would be gained by consulting the paper itself. On the other hand, material of great interest from other standpoints may be ignored entirely, or dismissed in a few indicative words. The report of a short structural paper is occasionally longer than the paper itself, interatomic distances, say, having been added by the abstractor; long papers mainly of chemical/ metallurgical or mineralogical interest may be represented merely by quotation of a cell dimension. The minimum criterion for the preparation of a report is ordinarily that the paper contains the determination or more accurate redetermination of a unit cell, but investigations of texture, papers containing powder data, and electron-diffraction studies have been reported when of some structural interest. Papers of this type in Russian and other journals not readily available have been included more freely than those in easily accessible sources.

The arrangement within individual reports is usually Name, Formula, Papers reported, Unit cell, Space group, Atomic positions and parameters, Interatomic and intermolecular distances, Material, Discussion, Details of analysis, References. The first, third and last of these are invariable, but deviations in the order of the rest occur whenever a gain in brevity or clarity is achieved. Editorial comments are enclosed in square brackets; it may be assumed that material not distinguished in this way is based directly on the papers reported.

This volume of *Structure Reports* is divided into three main sections: Metals, Inorganic Compounds, Organic Compounds. In the Metals section the arrangement is alphabetical; details are given on p. 2.

No simple alphabetical arrangement seemed practicable for the Inorganic and Organic sections. Classification according to structure type also seemed impracticable, and was in fact falling into disuse in the later volumes of *Strukturbericht*. Reports in these sections, therefore, are placed roughly in order of increasing complexity of composition, related substances and related structures being kept together as far as possible. Inorganic and organic compounds should be sought in the subject or formula index.

The subject index is arranged alphabetically by the names printed as the headings of reports, and some effort has been made to include other common names. It has not been possible to do this systematically, however, and if no entry is found for the name first thought of, search should be made under a reasonable alternative, or in the formula index. As a result of the experience gained in compiling vol. 14 some small improvements have been made in the subject index.

In the formula index the constituents are arranged in the *alphabetical order of the chemical symbols*; this is unique, and conventional orders such as the electrochemical series are likely to cause trouble to crystallographers not trained as chemists. At the request of certain organic chemists an additional index of carbon compounds is included, in which the primary classification is by the number of carbon atoms and the secondary classification is by the number of hydrogen atoms, without regard to the nature of the other atoms present.

The scheme of transliteration of Russian usually employed\* is reproduced on p. vi, and the usual abbreviations of journal titles are given on p. 592. Transliteration is in accordance with draft recommendation no. 6 of the International Organization for Standardization (which is, unfortunately, subject to revision), and the abbreviations are based on the World List of Scientific Periodicals.

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15 October 1959

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# STRUCTURE REPORTS

## *SECTION I*

# METALS

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## ARRANGEMENT

In the Metals section of *Structure Reports* the arrangement is strictly alphabetical, and metals and alloys are not included in the subject and formula indexes. Thus magnesium-copper alloys should be sought under **Copper Magnesium**, steels under **Carbon Iron** (not iron carbon), and solutions of hydrogen in tantalum under **Hydrogen Tantalum**. When there is a reasonable doubt whether a substance should be classed as a metal or as an inorganic compound a cross-reference is usually given, but this is not always practicable. To be sure that information regarding such substances is not overlooked, therefore, search should be made both in the appropriate place in the Metals section (for example, **Tellurium Vanadium**) and under the appropriate name in the subject index (for example, Vanadium telluride).

The names and spellings aluminum, beryllium, caesium, niobium, sulphur and wolfram should be noted.



## Aluminum

See also aluminum magnesium, p. 7 below, and pp. 382, 403.

- I. [Anomalous lattice constants of small crystals of certain metals.] N. A. ŠIŠAKOV, 1952. *Ž. Eksp. Teor. Fiz. SSSR*, **22**, 241—245.

The data of 1 on aluminum deposited on platinum (cathodically deposited on glass) were recalculated. It was found that both the intensities and the  $d$  values did not correspond very well to the tetragonal cell reported. The pattern could be adequately explained on the basis of two face-centred cubic cells,  $a = 3.94$  and  $a = 3.86$  Å. The dimensions are uncertain because the data were taken from 1 and the accelerating voltage was not known. It is probable that the larger cell is due to Al with  $a = 4.04$  Å. On this basis, the platinum phase has a dimension of  $a = 3.96$  Å, which is 1.5% bigger than for pure Pt with large crystal size.

By sputtering Pt on Al foil in a vacuum and dissolving most of the foil, a sample of Pt was obtained which could be calibrated by the Al not dissolved. An electron-diffraction pattern of this sample showed spots due to Al and rings due to Pt. Using 4.04 Å for Al, the cell dimension of Pt was calculated as 3.97 Å  $\pm$  1%. Hence Pt and not Al changes cell dimension with small particle size.

[See similar but more precise work on the change of cell dimensions with particle size under gold, p. 95, and silver, p. 137.]

1. G. J. FINCH and A. G. QUARRELL, 1933. *Proc. Roy. Soc.*, A **141**, 398; *Strukturbericht*, **3**, 201.

## Aluminum Arsenic Lithium

- I. Herstellung und Eigenschaften der Verbindungen  $\text{Li}_3\text{AlP}_2$  und  $\text{Li}_3\text{AlAs}_2$ . ROBERT JUZA and WERNER SCHULZ, 1952. *Z. anorg. Chem.*, **269**, 1—12.

### $\text{AlAs}_2\text{Li}_3$ AND $\text{AlLi}_3\text{P}_2$

*Orthorhombic* (slightly distorted  $\text{CaF}_2$  structure)

	Cubic			$D_m$	$Z$	$D_g$
	$a$	$b$	$c$			
	in Å [from kX]					
$\text{AlAs}_2\text{Li}_3$	11.886	12.003	12.136	12.00	2.99	16 3.04(8)
$\text{AlLi}_3\text{P}_2$	11.492	11.630	11.752	11.65	1.90	16 1.86(6)

*Space group*  $Ibca$  ( $D_{2h}^{27}$ )

Related to space group  $Ia3$  ( $T_h^1$ ) of the cubic structure.

### Atomic positions

Based on positions in  $Ia3$ , isomorphous with  $\text{AlLi}_3\text{N}_2$  (1).

16 Al in (c) with  $x = 0.121$

48 Li in (e); parameters not determined

•8 As (P) in (a)

24 As (P) in (d) with  $x_{\text{As}} = 0.233$ ;  $x_{\text{P}}$  assumed to have the same value

Corresponding positions in space group *Ibca*:

32 As or P in 8(a), 8(c), 8(d) and 8(e)

16 Al in 16(f)

48 Li in 16(f), three times

### *Materials, Details of analysis*

The samples were prepared in three ways:  $\text{AlLi}_3$  plus P (or As) heated at about  $700^\circ$ ,  $\text{Li}_3\text{P}$  (or  $\text{AsLi}_3$ ) plus AlP (AlAs) heated at about  $700^\circ$ ;  $\text{Li}_3\text{P}$ , Al plus P heated at  $650$ – $700^\circ$ .

Powder diagrams were made in 53.3- and 114.6-mm diameter cameras with  $\text{CuK}$  radiation. Cell dimensions were calculated only from lines which were clearly resolved. The atomic parameters were calculated on the basis of the cubic structure, taking intensities from powder diagrams in the small-diameter camera where the lines were not too well resolved. Trial and error calculations were made for about a dozen reflexions.

### 1. *Structure Reports*, 11, 21.

## Aluminum Cerium Silicon



I. See I of lanthanum silicon, page 105.

*Hexagonal*,  $a = 6.24 \text{ \AA}$ ,  $c = 7.30 \text{ \AA}$  [from kX],  $Z = 2$ .

### *Material*

The material was obtained by reaction of excess silicon with a molten alloy of cerium and aluminum, followed by leaching with sodium-hydroxide solution. Chemical analysis corresponded to  $\text{Al}_3\text{Ce}_2\text{Si}_2$  rather than to the expected  $\text{CeSi}_2$ . [No details of the X-ray methods are given.]

## Aluminum Chromium

I. Die Auswirkung extrem hoher Abkühlungsgeschwindigkeit auf die Erstarrung und das Gefüge binärer Legierungen. GÜNTER FALKENHAGEN and WILHELM HOFMANN, 1952. *Z. Metallk.*, 43, 69–81.

Severely quenched alloys were examined by the back-reflexion method to determine from the cell dimensions the extent to which the solute could be maintained in solution. The results, given graphically, are listed in the table below, in which the equations of the straight lines representing the lattice parameters *versus* composition are given. The dimensions have been converted to  $\text{\AA}$  from kX.

System	Cell dimensions Face-centred-cubic cell	Extent of solubility in quenched specimens	Equilibrium solubility
Al—Cr	$4.0497 - 0.00828 (\text{at. \% Cr})$	2.85 at. % Cr	0.45 at. % Cr
Al—Mn	$4.0497 - 0.00647 (\text{at. \% Mn})$	4.7 at. % Mn	0.7 at. % Mn

System	Cell dimensions Face-centred-cubic cell	Extent of solubility in quenched specimens	Equilibrium solubility
Al—Ti	4.0497 — 0.0106 (at. % Ti)	0.19 at. % Ti	0.09 at. % Ti
Al—V	4.0500 — 0.00739 (at. % V)	0.55 at. % V	0.18 at. % V
Ca—Pb	4.9502 — 0.00179 (at. % Ca)	0.95 at. % Ca	0.52 at. % Ca
Cr—Cu	3.6152 + 0.0892 (at. % Cr)	1.8 at. % Cr	0.9 at. % Cr
Pb—Na	4.9510 — 0.00278 (at. % Na)	23.8 at. % Na	10.1 at. % Na
Pb—Te	4.9502 — 0.00512 (at. % Te)	0.32 at. % Te	0.16 at. % Te

The estimated accuracy of the cell dimensions is  $\pm 0.0003$  Å.

The alloys were cast into cooled copper moulds so that cooling rates up to  $25000^{\circ}$  per second could be obtained for the alloys while molten, and up to  $5000^{\circ}$  per second after solidification. The solvent metals, Al, Pb, and Cu had purities of 99.99%.

Back-reflexion diagrams were made with  $\text{CuK}\alpha$  radiation for the Al and Pb alloys;  $\text{CoK}\alpha$  radiation for the copper-chromium alloys.

### Aluminum Chromium Nickel

$\text{CrNi}_3$

$\text{AlCr}_4\text{Ni}_{15}$

- I. A study of order-disorder and precipitation phenomena in nickel-chromium alloys. 1952. A. TAYLOR and K. G. HINTON, *J. Inst. Met.*, **81**, 169—180.

Electrical resistivity, specific heat by the Sykes method, and X-ray diffraction studies by the Debye-Scherrer method were made on face-centred-cubic high-purity alloys having the compositions  $\text{Ni}_3\text{Cr}$  and  $\text{Ni}_{15}\text{Cr}_4\text{Al}$  and lying within the  $\gamma$  primary phase field of the Al—Cr—Ni system.

Well-defined superlattice lines indicative of long-range order are observed in  $\text{Ni}_{15}\text{Cr}_4\text{Al}$  but not in  $\text{Ni}_3\text{Cr}$ . However, changes in specific heat and electrical resistivity suggest that  $\text{Ni}_3\text{Cr}$  probably orders with the formation of antiphase domains or undergoes some increase in the degree of short-range order. The decrease in the  $\text{Ni}_3\text{Cr}$  lattice parameter from  $a = 3.5524$  Å for the alloy quenched from  $750^{\circ}$  to  $3.5518$  Å for a specimen slowly cooled over 6 days from  $900^{\circ}$  is in the right direction for an increase in the degree of order.

### Aluminum Cobalt Copper Iron Nickel

- I. Physical structure and magnetic anisotropy of Alnico 5. R. D. HEIDENREICH and E. A. NESBITT, 1952. *J. Appl. Phys.*, **23**, 352—365.

Heat-treated Alnico 5, of composition Ni 14% (weight), Al 8%, Co 24%, Cu 3%, Fe 51%, was studied by means of "electron metallography", a method that combines the techniques of electron microscopy and electron diffraction. It was concluded that the high coercive force of the alloy was caused by a very fine precipitate of a cobalt-rich face-centred-cubic transition structure with  $a = 10$  Å. This appears as rods 75—100 Å by 400 Å long spaced 200 Å apart

which grow along the [100] directions of the body-centred-cubic matrix crystal. Short arced rings for a structure not yet understood are also seen. This appears to be body-centred-cubic with  $a \sim 3.0$  Å. The structures of the electron micrographs are similar to the optical micrographs obtained by Bradley (1) for the Fe—Ni—Al system.

1. A. J. BRADLEY, 1952. *J. Iron St. Inst.* **171** (1), 41—47.

## Aluminum Copper

- I. See aluminum magnesium, II, p. 7 below, for reference, material, details of analysis.

No lattice parameters are quoted. Measured and calculated densities agree within the limits of experimental error.

- II. Interprétation de la diffusion anormale des rayons X par les alliages à durcissement structural. A. GUINIER, 1952. *Acta Crystallogr.*, **5**, 121—130.

- III. Formation et développement des zones et des précipités au sein des solutions solides sursaturées. *Idem*, 1952. *Z. Elektrochem.*, **56**, 468—473.

Previous experimental results (Al—Cu, Al—Ag, Al—Zn, Cu—Be) are reconsidered in light of the conflict of ideas of Guinier and Geisler and Hill (1). The ageing processes are grouped into a low- and a high-temperature region with a demarcation temperature around 200°C. It was concluded that the previous ideas of both Guinier and Geisler and Hill were incompatible with the experimental data and needed modification. At low temperatures zones of segregated atoms are formed, but if the size of the segregated atoms is considerably different from that of the matrix, the zones form irregular structures, distorted from the matrix, tending toward a structure different from that of the first precipitate. The zones are very numerous and coherent with the matrix. At higher temperatures the zones are no longer stable and ageing proceeds by the formation of nuclei of the precipitate and their subsequent growth.

- IV. [On the nature of natural ageing in aluminum alloys.] JU. A. BAGARJACKIJ, 1952. *Dokl. Akad. Nauk SSSR*, **87**, 559—562.

On the basis of data which he has obtained, the author supports the ideas of Guinier in contrast to those of Geisler and Hill.

1. *Structure Reports*, **11**, 22.

## Aluminum Copper Magnesium

- I. See aluminum magnesium, I, p. 7 below, for reference, materials, and details of analysis.

At. % Mg	At. % Cu	$a$ in kX at 25°C	At. % Mg	At. % Cu	$a$ in kX at 25°C
0.189	0.367	4.0397(9)	1.311	0.246	4.0450(4)
0.456	0.247	4.0415(7)	1.608	0.127	4.0468(2)
0.655	0.119	4.0428(4)	0.356	0.302	4.0409(0)

At. % Mg	At. % Cu	a in kX at 25°C	At. % Mg	At. % Cu	a in kX
0.202	0.880	4.0376(6)	0.578	0.179	4.0423(7)
0.414	0.750	4.0390(9)	1.058	0.422	4.0430(7)
0.637	0.628	4.0407(9)	0.570	0.659	4.0395(6)
0.927	0.500	4.0425(3)	0.804	0.521	4.0408(3)
1.247	0.362	4.0442(6)			

### Aluminum Copper Manganese

For  $\text{Al}_{20}\text{Cu}_3\text{Mn}_3$  see aluminum manganese nickel, p. 10 below.

### Aluminum Lithium Phosphorus

See aluminum arsenic lithium, p. 3 above.

### Aluminum Magnesium

See also magnesium, p. 108 below.

- I. Lattice-spacing relationships in aluminium-rich solid solutions of the aluminium-magnesium and aluminium-magnesium-copper systems. D. M. POOLE and H. J. AXON, 1952. *J. Inst. Metals*, **80**, 599—604, 1951—1952.
- II. Factors affecting equilibrium in certain aluminium alloys. E. C. ELLWOOD, 1952. *Ibid.*, 605—608.

*Cubic.* Measurements corrected to 25°C.

At. % Mg	a in kX	Ref.	At. % Mg	a in kX	Ref.
0	4.0412(1)	I	2.21	4.0494(3)	II
0.18	4.0415(7)	I	4.48	4.0595(8)	II
0.32	4.0422(4)	I	6.72	4.0695(0)	II
0.59	4.0427(3)	II	7.15	4.0723(5)	I
0.62	4.0434(4)	I	9.01	4.0797(8)	II
1.19	4.0444(6)	II	11.2	4.0908(1)	II
1.28	4.0460(3)	I	13.3	4.1002(1)	II
1.93	4.0489(2)	I	15.6	4.1092(5)	II

### Material

I. Aluminum of 99.991%, Mg of > 99.98%, and copper of 99.995% purity were melted together in alumina-lined crucibles and chill-cast in iron moulds. The ingots were annealed in evacuated glass tubes at 450°C for 7 days (binary alloys) or 10 days (ternary alloys), contamination from the glass being avoided by aluminum-foil wrappings. The outer portion of the ingot was removed, and about 1 gm of filings taken from the rest. The filings, protected by alumina, were again annealed in evacuated glass tubes at 450°C and quenched. Part of each lot of filings was analysed and part used for the X-ray measurements.

Slightly lower lattice parameters were obtained from a series of alloys prepared with Mg of lower purity.

II. Al 99.9985% pure, Mg 99.994%, Ag "spectrographically pure", 50 gm ingots. For Al—Ag and Al—Cu the ingots were analysed, but for Al—Mg it was necessary to analyse the actual filings. Annealing temperature 448°C for Al—Mg, 536°C for Al—Ag and 546°C for Al—Cu. Density measurements were made on portions of the ingots after hammering and further annealing.

#### *Details of analysis*

I. CuK radiation, 19-cm powder camera shielded from temperature fluctuations (variation  $< 0.4^\circ\text{C}$  during an exposure), Nelson-Riley extrapolation. No correction for refraction; measurements corrected to  $25^\circ\text{C}$  with an assumed value of  $\alpha = 23.1 \times 10^{-6}$  per  $^\circ\text{C}$ .

The value of  $a$  for Al is about 0.0001 kX lower than other recent measurements; this is attributed to variations in purity and poorer temperature control in previous work.

II. As I, except that a 9-cm camera was used. No details of temperature control.

#### *Lattice vacancies*

II. The measured densities are all rather less than those calculated from the lattice parameters. Interpretation in terms of vacant lattice sites is given in fig. 1.

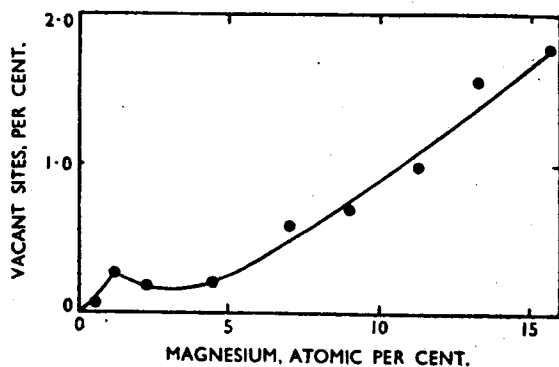


Fig. 1. Vacant lattice sites in the Al—Mg system (II).

An interpretation in terms of Brillouin zones is offered.

III. Étude aux rayons X de l'évolution des alliages aluminium-magnésium à 7% de magnésium au cours du revenu. A. R. WEILL, 1952. *Rev. metall.*, 49, 364—373.

A sample containing 8.38% Mg, 0.31% Mn, 0.38% Fe, 0.14% Si and 0.02% Cu

was aged at 160°. The lattice parameters of the solid solution were measured by the back-reflexion method (calibrated with Mo) during the course of the ageing (CoK radiation). The lattice parameters of the original solid solution dropped from a value of 4.0813 Å [from kX] (6.4% Mg) to about 4.0782 Å [from kX] (5.95% Mg) after ageing 428 hours. A new phase with  $a = 4.068$  Å [from kX] (4.0% Mg) appeared at this time. The lines were very diffuse at this stage. On continued ageing, the original solid-solution lines disappeared, the lines of the new phase sharpened, and the cell dimension continued to drop to 4.0624 Å [from kX] (2.7% Mg) after 2000 hours. The data indicate principally a discontinuous type of transition, but the diffuse character of the lines at about 500 hours of ageing may indicate a transition to a continuous transformation or severe lattice strains in the polycrystalline sample.

## Aluminum Magnesium Zinc

### Mg<sub>32</sub>(Al, Zn)<sub>48</sub>

- I. Crystal structure of the intermetallic compound Mg<sub>32</sub>(Al, Zn)<sub>48</sub> and related phases. GUNNAR BERGMAN, JOHN L. T. WAUGH and LINUS PAULING, 1952. *Nature, Lond.*, **169**, 1057—1058.

#### Cubic, body-centred

Cell dimensions are not given, but  $a = 14.16$  kX was found by 1 for Al<sub>2</sub>Mg<sub>3</sub>Cu<sub>3</sub>.

#### Space group $Im\bar{3} (T_h^5)$

##### Atomic positions (0, 0, 0; $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ ) +

2 Al in (a): 0, 0, 0 (12 near neighbours)

24 (Zn, Al: 83% Zn, 17% Al) in (g):  $\pm (0, y, z; \odot)$ ,  $\pm (0, y, \bar{z}; \odot)$ , with  $y = 0.097$ ,  $z = 0.157$  (12 near neighbours)

24 (Zn, Al: 44% Zn, 56% Al) in (g) with  $y = 0.195$ ,  $z = 0.310$  (12 near neighbours)

48 (Zn, Al: 48% Zn, 52% Al) in (h):  $\pm (x, y, z; \odot)$ ,  $\pm (x, \bar{y}, \bar{z}; \odot)$ ,  
 $\pm (\bar{x}, y, \bar{z}; \odot)$ ,  $\pm (\bar{x}, \bar{y}, z; \odot)$  with  $x = 0.160$ ,  $y = 0.190$ ,  $z = 0.400$  (12 near neighbours)

16 Mg in (f):  $\pm (x, x, x)$ ,  $\pm (x, \bar{x}, \bar{x}; \odot)$  with  $x = 0.185$  (16 near neighbours)

24 Mg in (g) with  $y = 0.300$ ,  $z = 0.115$  (16 near neighbours)

12 Mg in (e):  $\pm (x, 0, \frac{1}{2}; \odot)$  with  $x = 0.185$  (15 near neighbours)

12 Mg in (e) with  $x = 0.605$  (14 near neighbours)

#### Interatomic distances

(Al, Zn)—(Al, Zn) = 2.7 Å; (Al, Zn)—Mg = 3.0 Å; Mg—Mg = 3.1 Å.

#### Discussion of the structure

The structure was determined by the stochastic method. Each atom was assu-

med to have 12—16 ligates, the interatomic distances were assumed normal, the atoms were to form concentric polyhedral shells about 0, 0, 0 and  $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$  positions in such a way that atoms of each cell are located radially with respect to centers of polyhedral faces of the next inner shell.

The sequence then is the central atom, surrounded by an icosahedron (12 atoms), then a pentagonal dodecahedron (20 atoms), next an icosahedron with which the dodecahedron produces a rhombic triacontahedron. The fourth shell has 60 atoms above the triangular faces of the triacontahedron. These atoms are at corners of a truncated icosahedron which has 20 hexagonal faces and twelve pentagonal faces. Twelve atoms are added from the centres of the twelve hexagonal faces to produce 12 rhombic faces perpendicular to the cubic axes of the crystal.

These complexes of 117 atoms arranged about 0, 0, 0 and  $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$  share 72 outer atoms with neighbours so that the number of atoms per lattice point reduces to 81 or 162 per cube. The 12 rhombic faces are shared with neighbouring complexes along the cube edges; the 8 hexagonal faces are shared along body diagonals.

The ideal structure has the composition  $(\text{Al}, \text{Zn})_{48}\text{Mg}_{32}$ . There is 39.5% Mg in this structure. The ternary phase has a variable composition, but the Mg content is about 38%. Diffraction patterns of  $\text{Al}_6\text{CuMg}_4$  are similar (contains 36.4% Mg), so that Mg atoms probably occupy the same positions in both phases. The  $\alpha$  phase in the Al—Mn—Si system is structurally related. Preliminary work shows that there are 138 atoms per cube and that it is simple cubic. Phragmén (2) reported the composition as  $\text{Al}_{10}\text{Mn}_2\text{Si}$  and  $a = 12.65 \text{ \AA}$ .  $\text{Al}_{20}\text{Fe}_5\text{Si}_2$  with  $a = 12.55 \text{ \AA}$  was also reported by 2, and it forms solid solutions with  $\text{Al}_{10}\text{Mn}_2\text{Si}$ .

#### *Details of analysis*

Intensity data were obtained from single crystals. The rough structure obtained by the stochastic method was refined first by the Fourier method, then by the least-squares method ( $hk0$  data only) in which composition parameters were added to determine the fractional distribution of Al and Zn atoms over sites not occupied by Mg atoms.

1. F. LAVES, K. LÖHBERG and H. WITTE, 1935, *Metallwirtschaft*, **14**, 793; *Strukturbericht*, **3**, 391.
2. G. PHRAGMÉN, 1950. *J. Inst. Met.*, **77**, 489. *Structure Reports*, **13**, 15.

## Aluminum Manganese

See aluminum chromium, p. 4 above.

## Aluminum Manganese Nickel

- I. The unit cell and Brillouin zones of  $\text{Ni}_4\text{Mn}_{11}\text{Al}_{60}$  and related compounds. KEITH ROBINSON, 1952. *Phil. Mag.*, **43**, 775—782.



*Orthorhombic*

	<i>a</i>	<i>b</i>	<i>c</i>	<i>D<sub>m</sub></i>	<i>Z</i>
Al <sub>80</sub> Mn <sub>11</sub> Ni <sub>4</sub>	23.8 Å	12.5 Å	7.55 Å	3.62 ± 5 g/cm <sup>3</sup>	2
Al <sub>20</sub> Cu <sub>2</sub> Mn <sub>3</sub>	24.2	12.5	7.72	...	[6?]
Al <sub>24</sub> Mn <sub>5</sub> Zn	25.1	24.8	30.3	3.70 ± 2	[40?]

*Space group*

Al<sub>80</sub>Mn<sub>11</sub>Ni<sub>4</sub>: systematic absences indicate *Bb\*\**, so the possibilities are *Bbmm*, *Bbm2* and *Bb2m*.

Al<sub>20</sub>Cu<sub>2</sub>Mn<sub>3</sub>: the pattern is very similar, and presumably the space group is the same.

Al<sub>24</sub>Mn<sub>5</sub>Zn: systematic absences indicate *C\*\*\**.

*Material and Details of analysis*

Single crystals were supplied by G. V. RAYNOR. Weissenberg and oscillation photographs, MoK $\alpha$  radiation, estimated accuracy  $\frac{1}{2}\%$ . Al<sub>20</sub>Cu<sub>2</sub>Mn<sub>3</sub> shows reflexion twinning on {101}.

*Discussion*

The strong X-ray reflexions of Al<sub>80</sub>Mn<sub>11</sub>Ni<sub>4</sub> and Al<sub>20</sub>Cu<sub>2</sub>Mn<sub>3</sub> indicate a Brillouin zone bounded by {060}, {333}, {832}, {10, 3, 0}, {004}, {703} and {11, 0, 1}, containing about 1.83 electrons per atom (possible range 1.74 to 2.04). For Al<sub>24</sub>Mn<sub>5</sub>Zn the zone is slightly smaller. The agreement with valencies suggested by Raynor (Al = 3, Cu = 1, Mn = - 3.66, Ni = - 0.61; 1) is rather better than with bond-theory valencies.

1. G. V. RAYNOR, 1944. *J. Inst. Metals*, **70**, 531.

**Aluminum Manganese Silicon**Al<sub>9</sub>Mn<sub>3</sub>Si

I. The structure of  $\beta$  (AlMnSi)—Mn<sub>3</sub>SiAl<sub>9</sub>. KEITH ROBINSON, 1952. *Acta Crystallogr.*, **5**, 397—403.

*Hexagonal*

Specimen composition, at. %				<i>a</i>	<i>c</i>	<i>c/a</i>	<i>D<sub>m</sub></i>
Mn/Si	Mn	Si	Al	in Å			
6/1	21.08	5.68	73.24	7.519	7.768	1.0331	...
6/2	22.05	6.50	71.45	7.513	7.745	1.0308	3.74
6/3	21.21	7.26	71.53	7.509	7.736	1.0299	...
6/6	19.60	8.88	71.52	7.500	7.722	1.0297	...
Al <sub>9</sub> Mn <sub>3</sub> Si	23.1	7.7	69.2	...	...	...	...

*Space group C6/mmc (D<sub>6h</sub><sup>4</sup>)*

Space groups with the same characteristic absences but lower symmetry were investigated but did not lead to improved agreement.