STRUCTURE REPORTS

FOR 1956

Volume 20

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SYMBOLS

The letters a, b, c; α, β, γ are used consistently for the edges and angles of the unit cell. Other letters used consistently are as follows.

U	Volume of unit cell
D_m	Measured density in g/cm^3 or specific gravity
D_x	Density in g/cm^3 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, or reliability index
s, m, w, v, b	Strong, medium, weak, very, broad

LIMITS OF ERROR

Errors are generally quoted in units in the last place. Thus 4·8754 ± 3 means 4·8754 ± 0·0003, 4·87 ± 3 means 4·87 ± 0·03, and 4·875 ± 15 means 4·875 ± 0·015. Occasionally a very doubtful last digit is placed in parentheses.

TRANSLITERATION OF RUSSIAN

а	a	и	i	р	r	ш	š
б	b	й	j	с	s	щ	šč
в	v	к	k	т	t	ы	y
г	g	л	l	у	u	ъ	,,
д	d	м	m	ф	f	ь	'
е	e	н	n	х	kh	э	ė
ж	ž	о	o	ц	c	ю	ju
з	z	п	p	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 reporter; 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 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; but complete alphabetical cross-references are no longer given. It is therefore necessary to use the subject and formula indexes when seeking work on alloy systems.

No simple alphabetical arrangement seems practicable for the Inorganic and Organic sections. Classification according to structure type also seems 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.

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. 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 will be found in earlier volumes. Transliteration is in accordance with draft recommendation no. 6 of the International Organization for Standardization, and the abbreviations are based on the World List of Scientific Periodicals.

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Ottawa, Canada.
10 August 1963

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STRUCTURE REPORTS

SECTION I

METALS

EDITED BY
J. W. CHRISTIAN

WITH THE ASSISTANCE OF THE FOLLOWING REPORTERS

T. H. K. BARRON
G. A. BOOTSMA
G. J. BULLEN
L. D. CALVERT
A. HELLAWELL
J. W. MARTIN
G. NAGORSEN
S. OGAWA
J. SPREADBOROUGH

ARRANGEMENT

In contrast to previous volumes of *Structure Reports*, in Volume **19** and subsequent volumes the arrangement of the Metals section is no longer strictly alphabetical with cross references given under subject headings. **It is therefore essential now to make use of the Subject and/or Formula Indexes when seeking work on metals and alloy systems.** Apart from this important difference, the arrangement of the Metals section remains similar to that found in earlier volumes.

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

Aluminum

I. The thermal expansion of aluminium at low temperatures as measured by an X-ray diffraction method. B. F. FIGGINS, G. O. JONES and D. P. RILEY, 1956. *Phil. Mag.*, **1**, 747—758.

II. [Precision determination of polycrystalline lattice parameters with a back-reflexion X-ray camera of high resolving power.] M. A. GUREVIČ and B. F. ORMONT, 1956. *Ž. Tekh. Fiz. SSSR*, **26**, 1106—1112. [English Translation: *Soviet Physics; Techn. Physics*, **1**, 1081—1087].

III. Strukturuntersuchung an flächenhaften Proben in einer kleinen Zylinderkamera. H. WEYERER, 1956. *Z. angew. Phys.*, **8**, 135—139.

IV. See Bismuth II, p. 49.

V. An X-ray study of lattice vibrations in aluminum. C. B. WALKER, 1956. *Phys. Rev.*, **103**, 547—557. See also *Idem*, 1956. *Bull. Amer. Phys. Soc.*, **1**, 138.

VI. X-ray Compton scattering from aluminum. *Idem*, 1956. *Phys. Rev.*, **103**, 558—563.

CELL EDGE AT ROOM TEMPERATURE

There seems no reason to alter the accepted value (**1**). New determinations give the following values at 25°C.

I $a = 4{\cdot}04963 \pm 2$ Å
III $a = 4{\cdot}04142 \pm 9$ kX [4·04958 Å]
II $a = 4{\cdot}0510 \pm 2$ Å [from kX]

A refraction correction of 0·00003 Å was applied in I.

THERMAL EXPANSION

Lattice parameters given by I are tabulated below. Standard error is stated to be ± 0·00002 Å; temperature was constant to ± 0·04°K.

Temperature (°K)	a (Å)	Temperature (°K)	a (Å)
20·4	4·03186	85·7	4·03314
32·3	4·03191	106·2	4·03412
44·4	4·03201	115·2	4·03462
55·1	4·03219	125·0	4·03528
66·0	4·03239	298·7	4·04968
75·0	4·03271		

The thermal expansion coefficient in the range −46° to +102°C is given by IV as $24{\cdot}3 \times 10^{-6}$.

Materials and Details of analysis

Stated purities 99·99% (I, III) 99·999% (II). I used 19-cm camera, van Arkel

mounting, Nelson-Riley extrapolation. (11 lines measured). II used precision back-reflexion camera. III used 5·7-cm Debye-Scherrer camera with Bragg-Brentano focussing and $\sin^2\theta$ extrapolation. IV used a focussing camera. All with Cu$K\alpha$ radiation, III also with Cr$K\alpha$ and IV used Co$K\alpha$. [For comment on accuracy claimed, see **2**].

DIFFUSE SCATTERING

V, VI. The diffuse scattering of X-rays by single crystals of aluminum has been measured at 300°K along seven lines in reciprocal space, chosen so as to give the dispersion curves for lattice waves propagated along the [100], [110] and [111] axes. The method is similar to that of Jacobsen (**3**) for copper, but it is improved by calculating the second-order scattering correction from a more realistic model and by determining the correction for incoherent Compton scattering by direct measurement. In order to do this, measurements were made for $\sin\theta/\lambda$ between 0·3 and 0·6 Å^{-1} at 5°K and 300°K, and the Compton scattering found by a self-consistent separation. The measured intensity of Compton scattering was found to be considerably smaller than the theoretical values previously used, and none of the present theoretical expressions are considered reliable over a reasonable range of angles. The resulting dispersion curves agree to within at most a few per cent both with the elastic constants and with neutron-diffraction measurements (**4**) at short wavelengths.

The force constants of a model with interactions between first, second and third neighbours are chosen to give the best fit with the experimental dispersion relations, and a vibrational frequency distribution then calculated from this model, in which full account is taken of critical points in reciprocal space (**5**, **6**). Comparison with the experimental heat capacity (**7**) shows the need to take explicit account of anharmonicity in the theory of lattice vibrations at room temperature.

The Debye temperature factor was checked on a low-temperature spectrometer and found to be given by Θ (X-ray) = 402°K.

1. *Structure Reports*, **12**, 3.
2. W. Parrish, 1960. *Acta Crystallogr.*, **13**, 838.
3. E. H. Jacobsen, 1955. *Phys. Rev.*, **97**, 654.
4. B. N. Brockhouse and A. T. Stewart, 1955. *Ibid.*, **100**, 756.
5. L. van Hove, 1953. *Ibid.*, **89**, 1189.
6. J. C. Phillips, 1956. *Ibid.*, **104**, 1263.
7. W. F. Giauque and P. F. Meads, 1941. *J. Amer. Chem. Soc.*, **63**, 1897.

Aluminum Antimony

I. Étude par diffraction électronique de la formation des alliages aluminium-antimoine en couches minces. P. Michel, 1956. *C. R. Acad. Sci. Paris*, **243**, 2063—2065.

Films formed by simultaneously evaporating antimony and aluminum are amorphous but crystallize on heating to 200°C (20% Al) to 400°C (50% Al). At the stoichiometric composition of the compound AlSb, a diamond ($A4$) structure with

a = 6·10 Å forms after heating at 320°C for 1 hr; this transforms to the normal zinc blende ($B3$) structure with a = 6·11 Å after ½ hr at 450°C.

Aluminum Boron

AlB_2 F.W. = 48·62

I. The preparation of aluminum diboride, AlB_2. E. J. FELTEN, 1956. *J. Amer. Chem. Soc.*, **78**, 5977—5978.

Hexagonal, $C32$ type structure (**1**), $a = 3·009 \pm 1$ Å, $c = 3·262 \pm 1$ Å.

Material

A stoichiometric mixture of 99·5% powders in a graphite tube was heated at 800°C for several hr *in vacuo*.

Details of analysis

Geiger-counter diffractometer measurements were made with Cu$K\alpha$ radiation.

1. *Strukturbericht*, **4**, 121.

Aluminum Carbon Iron Nitrogen

nitrided steels

I. Das Auftreten eines Kubischen Nitrids in aluminiumlegierten Stählen. W. KOCH, C. ILSCHNER-GENSCH and H. ROHDE, 1956. *Arch. Eisenhüttenw.*, **27**, 701—706.

Samples of low-carbon steels containing from 0·005 to 0·75% Al were nitrided for 17 hr in ammonia at 600°C and then heated to red heat for 48 hours at 1000°C in ammonia. The more Al the steel contained the more N it took up; electrolytic separation gave a face-centred-cubic phase in addition to the known nitrides Fe_4N, Fe_2N and AlN. It is thought that this is a nitride of general formula M_xN where $x \approx 1$ and that Al or Cr play an important part in its structure. The lattice constant of this nitride varies from 4·10 to 4·17 Å. Steels with Cr or Mo have the nitride parameter larger, and those with Mn or Al have parameters nearer 4·10 Å.

Aluminum Chromium Nickel Titanium

I. Constitution of nickel rich quaternary alloys of the Ni—Cr—Ti—Al system. A. TAYLOR, 1956. *J. Metals, N.Y.*, **8**, 1356—1362.

[See **1**—**3** for previous work on the ternary systems.]

Six single-phase regions exist in alloys with > 50 at. % Ni annealed to equilibrium at temperatures up to 1150°C. These are

(1) the f.c. cubic primary solid solution in Ni (γ)
(2) the f.c. cubic ordered phase based on Ni_3Al (γ')
(3) the hexagonal c.p. compound η-Ni_3Ti
(4)—(6) the b.c. cubic phases β_1-NiAl, β_2-NiTi, and β_3-Ni_2TiAl

The extent of the γ phase increases as the temperature is raised, whilst that of the γ' phase decreases. The form of the quaternary tetrahedron was approximately

established at 750°C and 1000°C, and it was found that the tie lines in the phase fields containing any two of the phases γ, γ′, lie approximately in the pseudo-ternary system formed by the planar section through the compositions Ni_3Cr—Ni_3Al—Ni_3Ti. The phase boundaries of this pseudo-ternary system were established accurately at 750°C and 1000°C (Figs. 1 and 2). The suggested form of the

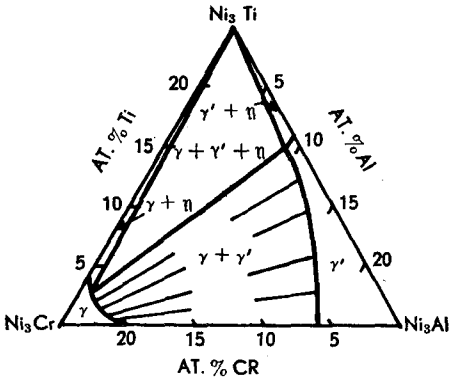

Fig. 1

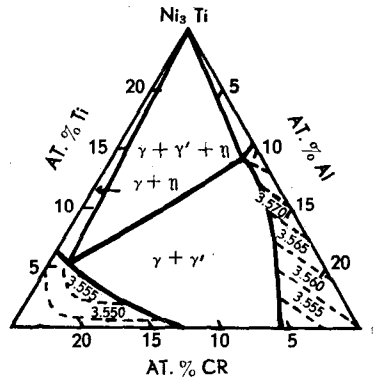

Fig. 2

Fig. 1. The Ni_3Cr—Ni_3Ti—Ni_3Al section of the Ni—Cr—Ti—Al system — 750°C isothermal.

Fig. 2. The Ni_3Cr—Ni_3Ti—Ni_3Al section of the Ni—Cr—Ti—Al system — 1000°C isothermal.

complete quaternary diagram includes a four-phase field linking the binary phases γ, γ′, and with the ternary Bertholide phase Ni_2TiAl. The structures of the alloys and lattice parameters of the main phases are shown in Table I.

Table I

Analysed composition (at. %)			Phases present		Lattice parameter after quench from 1000°C (Å [from kX])	
Cr	Al	Ti	1000°C	750°C	γ	γ′
22·0	1·2	1·4	γ	γ	3·5518	
21·0	2·2	1·6	γ	γ + γ′	3·5577	
21·0	1·6	2·6	γ	γ + γ′	3·5567	
20·4	3·8	0·8	γ	γ + γ′	3·5575	
19·8	4·3	1·3	γ	γ + γ′	3·5596	
19·9	2·4	2·6	γ	γ + γ′	3·5609	
18·9	5·2	0·7	γ	γ + γ′	3·5582	
18·7	4·8	1·3	γ	—	3·5592	
18·6	3·3	2·5	γ	γ + γ′	3·5623	
18·4	2·2	3·7	γ	γ + γ′	3·5630	
17·3	3·1	3·7	γ	—	3·5643	
15·4	7·4	1·4	γ	—	3·5598	
19·8	1·4	3·8	γ	γ + γ′	3·5580	

Analysed composition (at. %)			Phases present		Lattice parameter after quench from 1000°C (Å [from kX])	
Cr	Al	Ti	1000°C	750°C	γ	γ′
18·8	1·0	4·8	γ	γ + γ′	3·5650	
17·5	1·9	4·6	γ + γ′	γ + γ′	3·5644	
16·3	2·0	6·0	γ + γ′	γ + γ′	3·5641	
16·0	3·6	4·9	γ + γ′	γ + γ′	3·5660	
15·1	3·2	5·5	γ + γ′	γ + γ′	3·5670	
6·5	16·6	2·6	γ + γ′	γ + γ′		3·5646
1·4	11·2	12·3	γ + γ′	γ + γ′		3·5806
16·4	1·2	6·9	γ + γ′ + η	γ + γ′ + η	3·5675	
2·5	15·4	17·4	γ′	γ′		3·5738
2·6	19·6	2·5	γ′	γ′		3·5638
17·3	1·2	5·7	γ + η	γ + γ′ + η	3·5665	

Materials and Details of analysis

Most alloys were induction melted, Ti-rich alloys were melted in an argon-arc furnace. Main impurities were Ni—0·034% C, 0·018% Fe; Cr—0·15% Mn, 0·10% Al, 0·08% Fe, 0·01% Ni, Ti; Al—0·005% Fe; Ti—0·04% Mn, 0·015% Al, Fe.

Ingots were annealed *in vacuo* at 1200°C for 3 days and quenched.

Filings were cooled from 900°C—750°C in 4 days and then held at 750°C for 4 days before quenching.

Solid lumps were annealed 24 hr *in vacuo* at 1000°C and quenched, and filings then reheated to 1000°C for few minutes only. Debye-Scherrer photographs, Mn$K\alpha$ radiation.

1. *Structure Reports*, **16**, 57.
2. A. Taylor and R. W. Floyd, 1953. *J. Inst. Met.*, **81**, 25.
3. *Idem*, 1953. *Ibid.*, **81**, 451.

Aluminum Cobalt Copper
Aluminum Copper Iron

I. The structure of $FeCu_2Al_7$ and T(Co, Cu, Al). M. G. Bown and P. J. Brown, 1956. *Acta Crystallogr.*, **9**, 911—914.

Al_7Cu_2Fe

Tetragonal, $a = 6{\cdot}336 \pm 1$ Å, $c = 14{\cdot}870 \pm 2$ Å, $U = 597{\cdot}0 \pm 2$ Å^3, $D_m = 4{\cdot}30 \pm 8$, $Z = 4$, $D_x = 4{\cdot}44$.

The crystals were thin plates parallel to (001) and analysis gave Al: 50·7 wt %, Cu: 33·9 wt % and Fe: 15·4 wt %.

T(Al, Co, Cu)

Tetragonal, $a = 6{\cdot}3047 \pm 1$ Å, $c = 14{\cdot}756 \pm 1$ Å, $U = 586{\cdot}5 \pm 1$ Å^3, $D_m = 4{\cdot}0$—$4{\cdot}4$. Analysis gave Cu: $34{\cdot}3 \pm 1{\cdot}0$ wt%, Co: $13{\cdot}0 \pm 1{\cdot}0$ wt%.

The phases are isostructural and are described together.

Space group $P4/mnc$ (D^6_{4h}) and $P4nc$ (C^6_{4h}) are possible, $P4/mnc$ used (**2**)

Atomic positions

			Al_7Cu_2Fe	T(Al, Co, Cu)	S.D.
4 AlI	in 4(*e*):	with z =	0·1340	0·1320	± 8
4 Fe or Co	in 4(*e*):	with z =	0·2992	0·2970	3
8 Cu	in 8(*h*):	with x =	0·2780	0·2720	6
		y =	0·0880	0·0880	6
8 AlII	in 8(*g*):	with x =	0·1650	0·1530	20
16 AlIII	in 16(*i*):	with x =	0·1980	0·2020	20
		y =	0·4200	0·4200	20
		z =	0·1000	0·1000	8

Interatomic distances [Å]

		Al_7Cu_2Fe	T(Al, Co, Cu)
Cu:	2 Cu	2·613	2·549
	1 Cu	3·026	3·082
	2 AlIII	2·511	2·528
	2 AlIII	2·522	2·543
	2 AlIII	2·625	2·599
	2 AlI	2·717	2·652
Fe, Co:	4 AlIII	2·483	2·468
	4 AlII	2·477	2·489
	1 AlI	2·456	2·434

		Al_7Cu_2Fe	T(Al, Co, Cu)
AlI:	4 AlIII	2·985	2·976
	4 AlII	2·928	2·957
AlII:	2 AlIII	2·726	2·674
	2 AlIII	2·888	2·933
	2 AlIII	3·259	3·181
	1 AlII	2·957	2·728
	4 AlII	3·346	3·381
AlIII:	1 AlIII	2·706	2·740
	2 AlIII	2·799	2·754
	1 AlIII	2·974	2·951

Discussion

The structure, Fig. 1, may be described in terms of slabs and layers parallel to (001). The slabs consist of cubes of Al atoms, centred by Cu atoms, but with every fifth centrepoint unoccupied. Alternate slabs are displaced and rotated about the

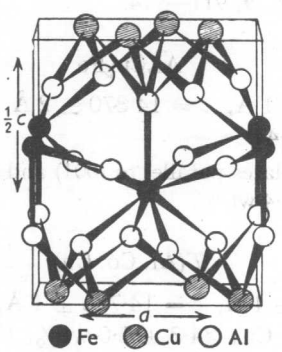

Fig. 1. One half of the unit cell of $FeCu_2Al_7$.

z axis. Between the slabs are flat layers of Al atoms in a square-and-triangle pattern. The Fe atoms are placed alternately just above and below the squares and are coordinated to 9 Al atoms. The nine-fold polyhedron around the Fe atoms has a square base, at the waist another larger square rotated with respect to the base, and a point at the top. A similar arrangement occurs in Co_2Al_9 (**5**). This structure was first given by **2**; the phase Al_7Cu_2Fe was found by **1** and its composition has been discussed in **3**. The most prominent Brillouin [Jones] zone has been calculated in **4** where it was shown that considerable overlap must occur for both phases. It is therefore probable that these phases should not be classed as electron compounds.

Details of analysis

For T(Al, Co, Cu) 63 ($h0l$) reflexions were observed (filtered Mo radiation) using a multiple-film Weissenberg technique. Corrections were made for Lorentz and polarization factors but not for absorption ($\mu_1 \sim 100\ cm^{-1}$). Starting from Westgren's parameters (**2**) the structure was refined by F_o and $F_o - F_c$ syntheses ($R = 0{\cdot}083$). Using data obtained with Co$K\alpha$ radiation, the Co atoms were located in sites 4(e) with $z = 0{\cdot}297$; random occupation of 8(h) and 4(e) by Cu and Co atoms was not compatible with the data. The discrepancy between the ideal formula Al_7Cu_2Co and the observed composition $Al_7Cu_{1{\cdot}9}Co_{0{\cdot}8}$ could neither be explained by a 20% deficiency in the Co sites ($R = 0{\cdot}135$), nor by moving the atoms. No definite replacement scheme could be decided on the data available.

For Al_7Cu_2Fe, a crystal $0{\cdot}01 \times 0{\cdot}004 \times 0{\cdot}004$ cm was used and a similar refinement technique followed. The final value of R was 0·081. Comparison of the intensities shows Al_7Cu_2Fe isostructural with T(Al, Co, Cu). The standard deviations of the coordinates for both phases are listed above.

1. *Strukturbericht*, **7**, 192.
2. *Structure Reports*, **13**, 8.
3. P. C. L. Pfeil and G. V. Raynor, 1949. *Proc. Roy. Soc.*, A **197**, 321.
4. P. J. Black, 1955. *Phil. Mag.*, (7), **46**, 401.
5. *Structure Reports*, **11**, 8.

Aluminum Cobalt Copper Iron Nickel

I. Reversibility of the coercive force in Alnico 5. M. G. van der Steeg and K. J. de Vos, 1956. *J. Appl. Phys.*, **27**, 1250.

Alnico 5 is 51% Fe, 24% Co, 14% Ni, 8% Al, 3% Cu. The effects of various heat treatments are quoted to support the view that different reactions take place during the two stages of the permanent magnet heat treatment designed to give high coercive force. In addition to the Fe—Co-rich precipitate, a new phase was detected after prolonged ageing (70 days) at 600°C. This phase has a face-centred cubic structure with a lattice parameter of 3·62 Å; it disappeared again on reheating to 820°C.

Aluminum Copper

AGE-HARDENING AL-RICH ALLOYS

I. The θ′ structure in aluminium-copper alloys. J. M. SILCOCK and T. J. HEAL, 1956. *Acta Crystallogr.*, **9**, 680.

II. Electroneninterferenz-Untersuchung an ausscheidungsfähigen Legierungen in dünner Schicht. I. Das System Aluminium-Silber II. Das System Aluminium-Kupfer. A. WINKELMANN, 1956. *Z. Metallk.*, **47**, 621—631.

I. Guinier's observation (**1**) that the intensities of diffraction spots for which $2h + l = 4n \pm 2$ are higher than expected from the distorted CaF_2-type structure (**2**) is confirmed. Observed intensities are compared with calculated intensities based on various models.

The best agreement was obtained with a structure in which approximately $\frac{1}{8}$ of the Al sites are vacant and 1 in 4 of the unoccupied sites of the Cu layer are filled with Al.

Details of analysis

Intensity data from single crystals, with focussed Mo$K\alpha$ radiation. Integrated intensities from sheet and rod specimens were corrected for absorption, geometrical factors and temperature.

II. Contrary to previous work on bulk specimens, it was found that the segregation and recrystallization in thin films of Al—Ag and Al—Cu alloys were already complete before the first observations could be made 20 minutes after quenching in the electron-diffraction apparatus.

COPPER-RICH ALLOYS

III. Construction et mise au point d'une chambre de precision pour diagrammes de rayons X à haute temperature. R. DIAMENT, 1956. *Métaux et Corros.*, **31**, 167—187.

Lattice parameters of an alloy with 11·89% Al, 0·005% Si, 0·001% Fe, 0·001% Mn.

α phase $a = 3{\cdot}668$ Å at room temperature
γ_2 phase $a = 8{\cdot}895$ Å at room temperature
β phase $a = 2{\cdot}947$ Å at 559—569°C.

The $\alpha + \gamma_2 \rightleftharpoons \beta$ eutectoid temperature was fixed at 559—569°C by high-temperature X-ray photographs in a Seeman-Bohlin-type camera.

1. *Structure Reports*, **9**, 5.
2. G. D. PRESTON, 1938. *Phil. Mag.*, **26**, 855.

Aluminum Copper Lithium

I. The phase sections at 500°C and 350°C of aluminium-rich aluminium-copper-lithium alloys. H. K. HARDY and J. M. SILCOCK, 1956. *J. Inst. Met.*, **84**, 423—428.

Three ternary intermetallic compounds T_B, T_1 and T_2 come into equilibrium with the aluminum solid solution at 500°C.

T_B ($\sim Al_{7\cdot5}Cu_4Li$)

Cubic Modified CaF_2 ($C1$) type structure. (**1**)

Composition (wt%)		a (Å)	Temperature (°C)	D_m
Cu	Li			
54·9	1·4	5·8328 ± 5	26	3·76
54·7	1·5	5·8325 ± 5	21	—
57·5	1·1	5·8255 ± 5	18	—
53·4	1·8	—	—	3·64

Neither sample used for density measurements was entirely T_B.

Unit cell composition	D_x
Al_7Cu_4Li	3·74
$Al_{7\cdot1}Cu_{3\cdot6}Li_{0\cdot9}$	3·55
$Al_{7\cdot2}Cu_{3\cdot84}Li_{0\cdot96}$	3·68
$Al_{7\cdot5}Cu_4Li$	3·85

The slight variation of a parameters may indicate a limited composition range. Calculated intensities for the ideal $C1$ structure $Cu_4(Al_7Li)$ are virtually identical with those for $Al_{7\cdot2}Cu_{3\cdot84}Li_{0\cdot96}$ in which a few Al atoms are exchanged for Cu atoms to fit the chemical analysis. Calculated intensities for other possible modifications $Al_{7\cdot1}Cu_{3\cdot6}Li_{0\cdot9}$ (vacancies in Cu positions) and for $Al_{7\cdot5}Cu_4Li$ (excess Al in Cu layers) are slightly different, but all agree reasonably well with observed intensities. The structure and parameter of T_B are both closely similar to those of the θ′ phase in aluminum-copper alloys.

T_1 (composition on Al-rich side of Al_2CuLi)

Hexagonal, $a = 4{\cdot}96$ Å, $c = 9{\cdot}35$ Å for a single crystal of 50·5 wt % Cu, 5·5 wt % Li. $a = 4{\cdot}96(6)$ Å, $c = 9{\cdot}34$ Å for 51·3 wt % Cu, 5·5 wt % Li.

Space group, *P*622, *P*6*mm*, *P*6*m*2, or *P*6/*mmm*, from absence of glide planes and screw axes. High-angle powder lines are weak; visual intensities are given for d values from 9·4 Å to 1·03 Å.

T_2 (composition on Al-poor side of Al_6CuLi_3)

Weak, "fairly simple", but not cubic powder pattern. Visual intensities and d spacings are given from 5·91 Å to 0·901 Å.

Three further intermetallic compounds, denoted P, Q and R, were found in alloys less rich in aluminum. P appeared in alloys with compositions close to T_B and had a powder pattern like T_1, but with changes in intensities and line shifts too great to be attributed only to a change of axial ratio. Metallographically P was similar to θ($CuAl_2$) in aluminum—copper alloys. Q was detected in high lithium alloys; the full powder pattern had many lines, and the phase reacted vigorously