STRUCTURE REPORTS

FOR **1957**Volume 21

GENERAL EDITOR

W. B. PEARSON

SECTION EDITORS

J. W. CHRISTIAN (Metals)
S. GELLER (Inorganic Compounds)
J. MONTEATH ROBERTSON (Organic Compounds)

PUBLISHED FOR THE

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

BY

N.V. A. OOSTHOEK'S UITGEVERS MIJ UTRECHT

First published in 1964

Copyright 1964 by the International Union of Crystallography. Short extracts and single illustrations may be reproduced without formality, provided that the source is acknowledged, but substantial portions may not be reproduced by any process without written permission from the International Union of Crystallography.

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.

\boldsymbol{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
\boldsymbol{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 Angström units
X', Y', Z'	Atomic coordinates in Angström 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 4.875 ± 0.003 , and 4.875 ± 15 means 4.875 ± 0.015 . Occasionally a very doubtful last digit is placed in parentheses.

TRANSLITERATION OF RUSSIAN

a	a	и	i	р	r	ш	š
б	b	й	j	c	s	щ	šč
В	v	ĸ	k	T	t ·	ы	y
r	g	л	1	У	u	ъ	
д		M	m	ф	f	ь	,
е	e	H	n	x	$\mathbf{k}\mathbf{h}$. 9	ė
ж	ž	0	0	ц	С	ю	ju
3	Z	п	р	ч	č	я	jaı

INTRODUCTION

The aim of Structure Reports is to present critical reports on all work of crystallographic structural interest, whether it is derived directly from Xray, electron or neutron diffraction, or even indirectly from other experiments. The reports are intended to be critical and not mere abstracts, except in some cases when a brief indication of the content of a paper of related interest is included in the form of an abstract. The length of a report may bear no relation to the length of the original publication. For example, the report of a brief note giving unit cell dimensions and structure type may be enlarged with information about space group and the calculation of interatomic distances, whereas a long paper dealing mostly with material of little crystallographic interest may be reported in a few words describing only the structural material given therein. In selecting topics for reporting, the criterion "of structural interest" is freely interpreted in terms of what is topically interesting. Thus, papers dealing with such subjects as cold-work, dislocations, twinning, or crystallinity, which once were reported, may no longer be in later years when topical interest in them has declined. Only in this way is it possible to keep yearly volumes of Structure Reports to a fairly uniform and usable size in view of the ever increasing amount of published material. Nevertheless, papers giving unit cell dimensions, space groups, and atomic coordinates are invariably reported if the material gives new or more accurate results than hitherto.

Ideally, the reports have been prepared in such a way that no further structural information would be gained by consulting the original paper itself. However, the rapidly increasing number of multi-parameter structures being determined, requires a change of this policy. Beginning with Volume 21, atomic parameters will no longer be reproduced for structures containing more than about 30 independent atoms. The reasons for this are mainly twofold: First, it is estimated that within a very few years Structure Reports would otherwise contain more than 100 pages of tables of atomic parameters alone. Secondly, it is considered that the chances of including typographical errors in reproducing these extensive tables of data are such, that anybody wishing to make detailed use of them would in any case consult the primary references.

Although the data in *Structure Reports* must be presented as briefly as possible, every effort is made to avoid jargon, so that the information is readily understandable by the non-crystallographer as well as by the crystallographer. Nevertheless it is assumed that the reader has available

Volume I of the *International Tables**, wherein he can obtain details of space group settings and equivalent positions of the atoms.

The arrangement in individual reports is generally: Name, Formula, Papers reported, Unit cell, Space group, Atomic positions, Interatomic and intermolecular distances, Material, Discussion, Details of analysis and References. Editorial comments are enclosed in square brackets, and it may be assumed that material not distinguished in this manner is based directly on the papers reported. The volume is divided into three main sections: Metals, Inorganic Compounds, and Organic Compounds. In the earlier volumes of Structure Reports the arrangement of the Metals section was strictly alphabetical, with crossreferences given in the text so that the preparation and use of an index to find data on alloys was unnecessary. In order to save space this practice was discontinued in Volume 18 and subsequently. Although the arrangement of the Metals section remains roughly alphabetical, it is now essential to use the Subject and Formula indexes when seeking work on elemental metals, intermetallic compounds and alloys. The arrangement of the Inorganic and Organic sections is roughly in the order of increasing complexity of composition, related substances and related structures being kept together as far as possible. Inorganic and organic compounds should therefore also be sought in the Subject or Formula indexes. The Subject index is arranged alphabetically by the names printed as the headings of the reports, and it also includes other common names and information. The Formula index is arranged in alphabetical order of the chemical symbols and is therefore unique. Double entries are made for organic compounds: i) strictly alphabetically, and ii) with C and H preceding other elements. A separate index of organic compounds is also included, in which primary classification is by the number of carbon atoms and secondary classification by the number of hydrogen atoms; other constituents then follow alphabetically. In these formula indexes solvents of crystallization follow at the end of the formulae, but double entries are frequently made, especially for inorganic compounds containing water, possibly or certainly as OH groups.

The scheme generally employed for the transliteration of Russian is reproduced on p. VI, and the usual abbreviations of journal titles are given on p. 660. 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.

• International Tables for X-ray Crystallography, Vol. I, Symmetry Groups. International Union of Crystallography, Kynoch Press, Birmingham, 1952.

W. B. Pearson

National Research Council, Ottawa, Canada. 20 September 1964

TABLE OF CONTENTS

List of symbols		•	•	•							•						•		VI
Introduction		•													•				VII
Metals				•	•,				•	•		í	٠.	•	٠		•		1
Inorganic Compo	und	s.		•										٠		•.			187
Organic Compour	ıds.		•									•	÷			•			495
Journal Abbrevia	tior	ıs		•					•		•	•	•.	•					660
Subject Index .			•								, •	•	٠,		. •	•			661
Formula Index.											•	٠.							678
Index of Carbon	Cor	mp	ou	ınd	ls						•	•	٠,•	•					687
Author Index	• •					•					•						•		689
Corrigenda															. •				706

STRUCTURE REPORTS

SECTION I

METALS

EDITED BY
J. W. CHRISTIAN

WITH THE ASSISTANCE OF THE FOLLOWING REPORTERS

G. B. BOKIJ

G. NAGORSEN

L. LEONARD

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 generally similar to that of earlier volumes.

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

Aluminum

I. [Determination of the atomic distribution functions in liquid Al and Bi at different temperatures from electron-diffraction photographs.] A. I. Bublik and A. G. Buntar', 1957. Fiz. Metall. Metalloved., 5, 53—57.

The first maximum in the atomic distribution function for liquid aluminum occurs at a radius of 2.7 Å, 2.94 Å and 2.98 Å at 670° C, 720° C and 850° C respectively, and corresponds to 11.4, 10 and 9 neighbours at this distance at the three temperatures. At 670° C the second maximum corresponds to a radius of 4.2 Å. The data were obtained from electron-diffraction photographs of thin films, $2-3 \times 10^{-6}$ cm in thickness. Experimental details are described in 1. The ordering just above the melting point approximates to that in the crystalline condition, but the density of atom packing decreases as the temperature is raised.

1. A. I. Bublik, 1957. Kristallografija, SSSR, 2, 249.

Aluminum Barium

I. Preparation and diffraction data of Ba—Al alloys. D. K. Das and D. T. PITMAN, 1957. J. Metals N.Y., 9, 1175.

Al₄Ba

Tetragonal, body centred (1), a = 4.566 Å, c = 11.250 Å.

Specimens were prepared from 99.9% Al and 99.5% Ba by induction melting under helium. The lattice spacings were determined from a diffractometer record using $CuK\alpha$ radiation. A table of d spacings and relative intensities is given.

1. E. Alberti and K. R. Andress, 1935. Z. Metallk., 27, 126.

Aluminum Cerium

I. Beitrag zur Kenntnis des Systems Cer-Aluminium. J. H. N. VAN VUCHT, 1957. Z. Metallk., 48, 253—258.

The system cerium-aluminum was investigated by thermal analysis, metallographic and X-ray methods over the range 0—50 at.% aluminum. Contrary to previous work (1), the only intermediate compound with less than 50 at.% aluminum is Ce₃Al. This exists in two allotropic modifications, the α form being stable below the transformation temperature of \sim 230°C [taken from the text; 250°C is shown in the phase diagram], and the β form being stable at higher temperatures.

Ce, quenched from 500°C, $a=5.162\pm1$ Å, U=137.55 ų, $D_x=6.77$. Ce, saturated with Al, $a=5.116\pm2$ Å [no further details.]

$$\alpha$$
-Ce₃Al F.W. = 447·37

Hexagonal, Mg₃Cd (D0₁₉) type (2), $a = 7.043 \pm 2 \,\text{Å}$, $c = 5.451 \pm 2 \,\text{Å}$, c/a = 0.774, $U = 234.16 \,\text{Å}^3$, Z = 2, $D_\alpha = 6.34$.

Space group $P6_3/mmc$ (D^4_{6h})

Atomic positions

6 Ce in 6(h): with x = 0.829 (ideally $x = \frac{5}{4}$). 2 Al in 2(c)

Interatomic distances (A)

Ce—6 Ce, 3.43 [in a sort of distorted trigonal prism, with Ce—2 Ce = 3.61 at the corners of an equilateral triangle.]

Ce—6 Al, 3.46, 3.70 [3.37 at the corners of a trigonal prism; 3.53 nearly hexagonal in a plane.]

β-Ce₃Al

Cubic, Cu₃Au (L1₂) type (3), $a = 4.985 \pm 1$ Å at room temperature in sample quenched from 500°C, U = 123.88 Å³, Z = 1, $D_x = 6.00$.

Interatomic distances (A)

Ce-12 Al, 3.53 [erroneously also given as Ce-Ce]

CeA1

F.W. = 167.11

Orthorhombic, a = 9.27 Å, b = 7.68 Å, c = 5.76 Å, $U = 410.08 \text{ Å}^3$, Z = 8, $D_x = 5.41$.

Space group Probably $Cmc2_1$ (C_{2v}^{12}) from absences. [or Ama2] A table of the powder lines and their intensities is given.

Materials and Details of analysis

The cerium contained 0.23 wt % Fe, \sim 0.7 wt % La, and much smaller amounts of Si, Mn, Mg and Ni; the aluminum was 99.998% pure. Alloys were arc melted under argon, powdered under toluene, and heat treated in vacuo. X-ray data are from diffractometer patterns with Mo radiation. The reliability factor for the structure of α -Ce₃Al was 0.14, including very weak reflexions. The equilibrium diagram shows negligible solubilities of either component in the compounds or in pure cerium. Ce₃Al melts at 655°C and forms eutectic mixtures with cerium and with CeAl.

- 1. M. Hansen, 1958. Constitution of Binary Alloys, p. 78. McGraw-Hill: New York.
- 2. Strukturbericht, 5, 7.
- 3. Ibid., 1, 486.

Aluminum Chromium Nickel Titanium

I. [The mechanism of structure transformations in age-hardening alloys based on nickel.] Ju. A. BAGARIATSKIJ and Ju. D. TIAPKIN, 1957. Kristallografija, SSSR, 2, 419—423. [1957, Soviet Physics: Crystallography, 2, 414—421.]

Age-hardening alloys of nickel containing 0—14% aluminum, 0—15% titanium and 0—22% chromium were investigated by X-ray oscillating crystal and diffuse scattering methods. After quenching from 1100—1250°C, all alloys showed the

presence of some superlattice domains of the Ni₈Al type, even when the equilibrium precipitate should be based on η -Ni₈Ti. The domain size was estimated to be between 40 Å and 400 Å in different alloys. The early stages of ageing at temperatures 600—800°C result in the progressive segregation of the solid solution into regions of different composition [spinodal type decomposition], with the period of the modulations \sim 300—400 Å. In many alloys, these segregates ultimately became precipitates of the $\gamma'(\text{Ni}_{8}\text{Al} \text{ phase})$, but in some alloys the Ni₈Al type ordering which formed in titanium-rich regions ultimately changed into hexagonal precipitates of the η phase. The η phase was oriented relative to the γ solid solution according to the relation $(00.1)_{\eta}$ // $(111)_{\gamma}$ and $(11.0)_{\eta}$ // $(110)_{\gamma}$.

Aluminum Chromium Nickel Titanium Wolfram

I. [A study of the solubility of titanium and the phase composition of the alloys of the quinary system Ni—Cr—W—Al—Ti.] I. I. KORNILOV, A. JA. SNETKOV and F. M. TITOV, 1957. Ž. Neorg. Khim., 2, 160—166.

Electrolytic residues from alloys of 20% Cr, 5% Al, 6% W and 3.25-8.2% Ti, balance Ni were found to contain a b.c. cubic (A2) phase with a=3.150 Å [from kX] for 3.25% Ti and a=3.139 Å [from kX] for 8.2% Ti. The phase is believed to be based upon a solid solution of chromium in wolfram. The alloys were annealed for 10 hr at 1130° C and air cooled.

Aluminum Cobalt Aluminum Nickel Carbon Titanium

I. The determination of the strength of the interatomic bond and the lattice distortion in the case of some Al- or Ti-containing compounds of high melting point and their solid solutions. J. S. UMANSKIJ and S. M. NIKOLAEVA, 1957. Acta Tech. Acad. Sci. Hungar., 18, 3—11.

Debye temperatures computed from relative X-ray powder line intensities at 110°, 295° and 473°K are given in the following table, together with r.m.s. amplitudes of atomic vibration at these three temperatures.

Alloy	Debye θ	R.m.s. amp	litude of vi	bration (Å)
(at. %)	(°K)	110° K	295°K	473°K
50 Al—50 Co	540	0.083	0.112	0.141
45 Al—55 Co	480	0.089	0.125	0.155
55 Al—45 Ni	420	0.097	0.141	0.176
50 Al—50 Ni	500	0.085	0-122	0-151
40 Al60 Ni	450	0.091	0-150	0.162
50 Ti50 C	1130	0.073	0.085	0.098
70 Ti30 C	840	0.076	0.094	0.112

Aluminum Cobalt Copper Nickel

 [On the variation of lattice constants of aged Al-bronze containing Ni and Co.] S. Suzuki, S. Matsuo and M. Yanagisawa, 1957. Rep. Gov. Ind. Res. Inst., Nagoya, 6, 625—628.

The change of lattice parameter with ageing time [estimated by reporter from published curve] for two aluminum bronzes is listed in the following table. Specimen 1 contained 6.0 wt % Cu and 1.06 wt % Co; specimen 2, 6.0 wt % Cu, 3.35 wt % Ni and 1.15 wt % Co. The increase in lattice parameter was found to take place in the initial stages of ageing, before maximum hardness was reached, and the ageing rate was decreased by additions of Zr and Ti. Lattice parameters are from powder photographs with $CuK\alpha$ radiation.

Ageing time (hr)	Lattice parameters (Å)					
at 500°C	Specimen 1	Specimen 2				
0	3-643	3-637				
0.5	3.648	3.643				
1	3.649	3.645				
3	3.646	, 				
5	3.643	3.642				
10	3.644	3.643				
40	3.646					
50	_	3.640				
100	3.647	_				
150	3.649	3.646				
200	· · · · · ·	3.644				
300	_	3.642				

Aluminum Copper

ALUMINUM-RICH ALLOYS

I. The structure of Guinier-Preston zones. II. The room-temperature ageing of the Al—Cu alloy. K. Toman, 1957. Acta Crystallogr., 10, 187—190.

The structure of the Guinier-Preston zone formed on ageing an alloy with 3.95% Cu at room temperature for ten days was determined by X-ray methods, following an earlier analysis of the diffuse diffracted intensity (1). In the following table, m_r is the atomic fraction of copper in the rth plane of the zone, and ε_r is the displacement of the rth atomic (001) plane from its position in the matrix.

7	m_{τ}	ε, (Å)	7	m_{τ}	ε, (Å)
0	0.98	0.00	6	0.13	
1	0.50	-0.0788	7	0.09	
2	0.39	-0.0311	8	0.06	_
3	0.30	-0.0069	9	0.04	_
4	0.23	-0.0006	10	0.025	
5	0.175	_			

The zone is thus a disc-shaped region consisting of a few atomic (100) planes in which the concentration of Cu decreases quite rapidly in both directions from the central atomic plane. The displacements of the planes in the centre of the zone do not reach the magnitude expected from the atomic radii of Cu and Al, but this is expected since the zone is coherent with the matrix. The structure differs from that of Gerold (2), in which the copper atoms segregate only to the central plane, and the displacements are larger.

Materials, Details of analysis

Single crystals were prepared from high purity wires of 1 mm diameter, and were aged at room temperature for ten days after quenching from 520°C. The aged crystals were etched in sodium hydroxide solution at 30°C. Weissenberg patterns were obtained with CuKa radiation, monochromatized with a bent quartz crystal. The diffuse intensity 00l was measured with a microphotometer for continuous variation of l from 1 to 5; interpolation had to be used near the Bragg maxima 002 and 004. The diffuse intensity was regarded as a trigonometrical series with the coefficients dependent on the structure of the zone, and these coefficients were obtained by a Fourier transform of the measured intensity, corrected for polarization, Lorentz and absorption factors. A least-squares procedure was used to find the structure summarized above. A final comparison of measured and calculated diffracted intensity shows good agreement over the whole range of l. This contrasts with Gerold's model, which gives good agreement near 002, but unsatisfactory agreement near 004. Since Gerold assumed that the Cu atoms segregate only to the central plane, and then found displacements to give best agreement with observed intensities, the present model is believed to be more accurate. The assumptions made are that Guinier-Preston zones may be regarded as twodimensional independently diffracting structures, and that all the diffuse intensity is due to the diffraction by the zones. If these assumptions are correct, the proposed structure is stated to give the best agreement between observed and calculated diffuse intensity.

- 1. Structure Reports, 19, 18. (VIII).
- 2. V. GEROLD, 1954. Z. Metallk., 45, 593; Structure Reports, 18, 17.

Aluminum Copper Iron Nickel

I. Aluminium rich alloys of the quaternary system aluminium-iron-coppernickel. G. V. RAYNOR and B. J. WARD, 1957. J. Inst. Met., 86, 135—144.

Figs. 1 and 2 show isothermal sections of the quaternary diagram at 530°C and total solute concentrations (copper + iron + nickel) of 10% and 15% respectively. In the composition range investigated, the Al solid solution exists in equilibrium with CuAl₂ and with the ternary compounds T-(FeCu) and T-(NiCu). T-(FeCu) has the approximate composition FeCu₂Al₇ and dissolves up to ~ 6.5 wt % Ni (replacing the Fe atoms) in the quaternary alloys. T-(NiCu) has approximate composition NiCu₂Al₆ and only dissolves ~ 0.8 wt % Fe.

Materials, and Details of analysis

Alloys were prepared from super-pure Al (99.997%) and master alloys. The

8 METALS

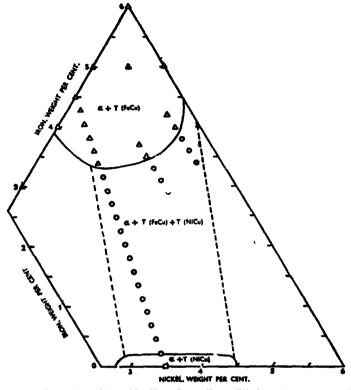
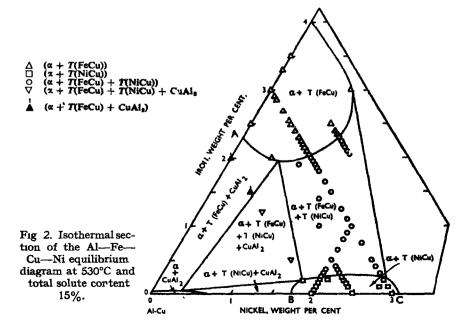


Fig. 1. Isothermal section of the Al—Fe—Cu—Ni equilibrium diagram at 530°C and total solute content 10%.



equilibrium diagram was determined from metallographic, X-ray diffraction and electrode-potential measurements. X-ray methods were used for phase identification of annealed samples, and of electrolytically extracted intermetallic compounds. $CuK\alpha$ and $CoK\alpha$ radiation.

Aluminum Copper Nickel

Crystal structure changes in the τ-phase of aluminum-copper-nickel alloys.
 S. S. Lu and T. Chang, 1957. Scientia Sinica, 6, 431—462 [Published in Chinese in Acta Physica Sinica, 1957, 13, 150—176.]

The limits of the ternary phase τ were re-investigated by X-ray methods, and some modifications are made to the earlier phase diagram of 1. X-ray powder patterns of the phase all show lines corresponding to the ordered CsCl (B2) type structure, but the lines are split, and additional lines are present. These additional lines undergo anomalous displacements as the composition is varied. An analysis of the patterns suggests that various structures exist within the phase, all being derived form a distorted CsCl cell which forms a basic rhombohedron. This cell has an aluminum atom at the corners and a heavy atom or a vacancy at the centre. The various structures are superstructures of the basic structure, and it is convenient to refer this to hexagonal axes in the usual way. The superstructure cells are then formed by stacking together the prismatic cells along the c axis, and the following structures are proposed.

Atomic compn		Type	Hex. s	ub-cell	True unit cell			
A1	Cu	Ni		a_0 (Å)	c_0 (Å)	a	c	
57	37	6	$ au_{\delta}$	4.1119	5-0250	a_0	$5 c_0 (10 c_0)$	
57	35	8	$ au_{11}$	4-1141	5.0263	a_0	11 c ₀	
57	34	9	τ_{6}	4.1132	5.0225	a_0	$6 c_0 (12 c_0)$	
57	32	1,1	$ au_{13}$	4-1133	5.0133	a_0	13 c_0	
61	28	11	$ au_{7}$	4.1062	4.9912	a_0	$7 c_0 (14 c_0)$	
60	28	12	τ ₁₅ .	4.0958	4.9763	a_0	15 c ₀	
61	27	12	τ_8	4.1045	4.9812	a_0	$8 c_0 (16 c_0)$	
61	26	13	$ au_{17}$	4.1014	4-9705	a_0	17 c ₀	

The number of units in these structures (the stacking number n in what follows) increases systematically from 10 to 17, the true unit cell being halved when this number is even. In general, this large cell is the primitive cell for the structure, but the symmetry is rhombohedral when n=3m-2 and m=4, 5 or 6. This means that τ_5 , τ_{13} and τ_8 have true unit cells which are rhombohedrons, as follows:—

$$\tau_5$$
: $a_R = 8.7050 \text{ Å}$, $\alpha = 27^{\circ}19'22''$
 τ_{13} : $a_R = 21.8537 \text{ Å}$, $\alpha = 10^{\circ}48'0''$
 τ_8 : $a_R = 13.4929 \text{ Å}$, $\alpha = 17^{\circ}29'50''$

 τ_8 is stated to correspond to the T_1 structure described by Bown (2), and it is also claimed that Bown's T_2 corresponds to τ_5 for the special case in which the angle of the basic rhombohedron approaches 90°. The value of n depends on the Ni and Cu content of the alloy; for constant Al content, it increases with increase in Ni

10 METALS

content. It is stated that the change in unit cell with composition is abrupt at certain compositions.

The following table gives the variation of the cell dimensions of the basic rhombohedron, together with measured densities and average number of atoms per unit cell.

Atomic compn.		Rhom	b. sub-cell	D_m	No. of atoms	
Al	Cu	N	a_r (Å)	α		in sub-cell
55	38	7	2.908	90°06′04″	5-07(1)	1.75(3)
55	37	8	2.906	90°07′20″	5.09(4)	1.76(0)
55	36	9	2.907	90°08′54"	5.13(5)	1.77(7)
55	35	10	2-907	90°09'34"	5-14(5)	1.78(4)
57	36	7	2.906	90°05′22″	4.89(9)	1.72(0)
5 7	35	8	2.907	90°05′42″	4.92(0)	1.73(0)
57	34	9	2.906	90°06′52″	4.92(6)	1.73(3)
57	33	10	2.905	90°09′46″	4.95(9)	1.74(6)
59	33	8	2.903	90°06′40″	4.75(5)	1-69(6)
59	32	9	2.902	90°10′22″	4.76(8)	1.70(1)
59	31	10	2.902	90°13′06″	4-79(8)	1.71(2)
59	30	11	2.898	90°18′02″	4.80(4)	1-71(2)
61	29	10	2.897	90°14'22"	4.65(3)	1.68(2)
61	28	11	2.896	90°17′14″	4.66(3)	• 1.68(9)
61	27	12	2.894	90°20′50″	4.68(6)	1.69(2)

In the ideal deformed CsCl structure, the number of atoms in a sub-cell is 2, whereas in the δ -phase, Ni₂Al₃ (D5₁₃) type structure (3) it is 1.666. The τ structures thus appear to be of the defect lattice type, with the number of defects smaller than in Ni₂Al₃.

Structures are proposed for the τ phase in which the original body-centre positions along all three triad axes are partially unoccupied, in contrast to the δ -phase, where the vacancies occur only along one triad axis. The proposed sequence of heavy atoms and vacancies in the centre positions along a triad axis, and the corresponding ideal formulae, are given below. The corner positions are assumed to be all occupied by aluminum atoms.

Structure	Occupation of "centre" positions by atoms (A) and vacancies (v)	Ideal Formula
$ au_{5}$	3A + 2v	Al ₅ (Cu, Ni) ₃
τ ₁₁	3A + 3v + 3A + 2v	Al ₁₁ (Cu, Ni) ₆
τ ₆	4A + 2v	Al ₆ (Cu, Ni) ₄
τ ₁₃	4A + 3v + 4A + 2v	Al ₁₃ (Cu, Ni) ₈
τ,	5A + 2v	Al ₇ (Cu, Ni) ₅
τ ₁₅	5A + 3v + 5A + 2v	Al ₁₅ (Cu, Ni) ₁₀
τ ₈	6A + 2v	Al _s (Cu, Ni) ₅
τ ₁₇	6A + 3v + 6A + 2v	Al ₁₇ (Cu, Ni) ₁₂

Examination of alloys quenched from 500°, 680° and 750°C respectively shows

that the rhombohedral angle decreases towards 90° as the temperature is raised. The intensities of the superstructure lines were not much affected by quenching from 500°C, but were markedly reduced in alloys quenched from above 680°C.

Materials and Details of analysis

Alloys were prepared by induction melting in vacuo from 99.992% Al, 99.999% Cu and 99.99% Ni; 58 alloys were prepared in all. Structural data are from powder photographs with $CoK\alpha$ radiation.

- 1. A. J. Bradley and H. Lipson, 1938. Proc. Roy. Soc., A, 167, 421.
- 2. Structure Reports, 20, 13.
- 3. Strukturbericht, 5, 10.

Aluminum Copper Titanium

I. Über eine aushärtbare Kupfer-Titan-Aluminium Legierung. W. GRUHL and H. CORDIER, 1957. Metall., 11, 928—933.

Age-hardenable alloys of Cu with 0.6-2.0% Ti and 0.45-1.2% Al were aged at $300-400^{\circ}$ C after a solution treatment at 800° C, and the precipitation process was followed by measurements of electrical and mechanical properties. Below 500° C, the precipitate which forms has a body-centred tetragonal cell with a=3.55(8) Å, c=4.62(5) Å, c/a=1.34; the composition of the phase is not known. Above 500° C, a second phase appears and is probably Cu_3 Ti. This has a slightly distorted hexagonal close-packed structure with a=2.619 Å, c=4.34(7) Å, c/a=1.66. X-ray data are from powder photographs with Co radiation.

Aluminum Indium Titanium

 Hexagonale Ordnungsphase in den Systemen Titan-Aluminium und Titan-Indium. K. Anderko, K. Sagel and U. Zwicker, 1957. Z. Metallk., 48, 57— 58.

In the binary system aluminum-titanium, the authors distinguish the phases α (0—10 at.% Al), α_2 (19—25 at.% Al) and Σ (28 at.% Al) instead of the single α solid solution of 1. A hexagonal superstructure of the Mg₃Cd ($D0_{19}$) type (2) forms a continuous solid solution from Ti₃Al to Ti₃In; the superstructure lines vanish at the composition Ti₃In_{0.25}Al_{0.75} as the scattering power of Ti lies between that of In and Al. There is possibly also a Ti₇Al phase, of space group $P\delta m2$ (D_{3h}^1). See also 3.

- 1. M. HANSEN, 1958. Constitution of Binary Alloys, p. 139.
- 2. Strukturbericht, 5, 7.
- 3. Structure Reports, 15, 13; 16, 15.

Aluminum Iridium and other Intermediate Phases.

I. Zur Systematik der Strukturfamilie des NiAs. P. Esslinger and K. Schu-Bert, 1957. Z. Metallk., 48, 126—134.

This is a survey of compounds of type TB where T is a transition metal (Cr to Cu