

Table 5.  $\Delta/\sigma$  values for the temperature coefficients

	$\Delta/\sigma (b_{11})$	$\Delta/\sigma (b_{22})$	$\Delta/\sigma (b_{33})$	$\Delta/\sigma (b_{12})$	$\Delta/\sigma (b_{13})$	$\Delta/\sigma (b_{23})$
Cu	-18.75	1.42	-11.00	1.06	-8.94	0.71
S(1)	-7.61	1.77	-6.38	-0.51	-5.70	0.00
S(2)	-10.53	4.91	-6.38	-0.40	-4.75	-0.89
S(3)	-6.68	4.24	-2.84	0.69	-0.49	-0.28
S(4)	-11.71	1.34	-5.68	-0.60	-6.33	-0.45
N(1)	-4.23	0.53	-2.01	2.60	-0.99	-0.49
N(2)	-3.14	0.58	-2.22	2.10	-1.02	-1.38
C(1)	-2.73	2.71	-1.57	-0.45	-0.09	-1.40
C(2)	-2.86	1.54	-1.64	1.04	-2.63	-0.66
C(3)	-2.18	-0.07	-0.45	-1.15	-0.26	-0.61
C(4)	-2.75	1.06	1.09	-0.89	0.19	-0.32
C(5)	-0.04	-0.49	-2.83	-1.26	-1.02	-0.91
C(6)	-2.30	2.21	-2.24	-0.43	-0.83	-0.64
C(7)	-1.66	1.53	-3.53	1.25	-1.61	-0.45
C(8)	-2.86	2.54	-2.04	1.84	-1.31	0.00
C(9)	-2.87	0.61	-1.11	1.29	-2.60	0.36
C(10)	-1.35	1.06	-0.11	-0.56	0.27	-0.22

The case is similar to others discussed recently by O'Connell (1965) who has shown that systematic errors in the intensity data or a poor choice of weighting function in the refinement may give rise to apparently significant differences from the correct structure. This results from the lack of validity of the assumption, made in assessing the standard deviations from the least-squares matrix, that the errors are predominantly random in character. O'Connell has shown that systematic data errors can arise from a tendency to overestimate the strengths of the weaker spots in photographic data. Although the errors in the individual measurements are small they result in film-factor errors which are cumulative, giving rise to large inaccuracies in the stronger intensities.

A comparison of the intra-pack film factor calculations for the model B data with more recent measurements by a photometric technique suggests that the film factors were slightly underestimated, but it is impossible to verify this by remeasurement of the original films because of the irregular spot shape. Moreover this type of error cannot account for all the discrepancies in the  $b_{ij}$ 's, since the  $\Delta b_{22}$ 's are in the opposite direction to that required. It may well be that the difference in the  $b_{ij}$ 's and the errors in the parameter standard deviations result from a combination of differing crystal disorder, absorption effects and film factor

and spot shape errors. It is clear, however, that little attention can be paid to the absolute magnitude of the  $b_{ij}$ 's, and that the standard deviations in the positional parameters must be regarded as an under-estimate. It seems probable, moreover, that errors of the type discussed above are by no means uncommon in structure analysis.

We wish to thank Professor A. Vacigo for some valuable discussions and, together with his colleagues, for conducting the least-squares refinement. One of us (B.H.O'C) is indebted to I.C.I. (Australia and New Zealand) for a research fellowship.

#### References

- BONAMICO, M., DESSY, G., MUGNOLI, A., VACIAGO, A. & ZAMBONELLI, L. (1965). *Acta Cryst.* **19**, 886.  
 BUSING, W. R. & LEVY, H. A. (1957). *Acta Cryst.* **10**, 180.  
 DAUBEN, C. H. & TEMPLETON, D. H. (1955). *Acta Cryst.* **8**, 841.  
 DOMENICANO, A., VACIAGO, A. & ZAMBONELLI, L. (1966). Personal communication.  
*International Tables for X-ray Crystallography* (1962). Vol. 3, p.201. Birmingham: Kynoch Press.  
 O'CONNELL, A. M. (1965). Personal communication.  
 RAE, A. I. M. (1963). Personal communication.

*Acta Cryst.* (1966). **21**, 830

#### X-ray powder data of $T$ phases composed of aluminum and magnesium with silver copper or zinc. By J. H.

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(Received 7 June 1966)

Ternary compounds designated  $T$  phases are found in age hardening alloys of aluminum and magnesium with silver, copper or zinc. These phases have a body-centered cubic lattice with a parameter of about 14 Å. The structure of the  $T$  phase in the Al-Mg-Zn system has been determined by Bergman, Waugh & Pauling (1957) who showed it to contain 162 atoms per unit cell corresponding to the formula  $Mg_{32}(Al,Zn)_{49}$ . The corresponding phase containing copper has been given the formulae  $Mg_4CuAl_6$  (Laves,

Löhberg & Witte, 1935) and  $Mg_4CuAl_5$  (Nishimura, 1937) based on approximations to composition. In investigations of the effect of silver additions to aluminum-magnesium alloys, a  $T$  phase has also been found in this system by Wheeler, Blankenburgs & Staddon (1965) and independently by ourselves; in each case compositions made to the formula  $Mg_4AgAl_6$  were not entirely single-phase.

As powder data were required by us for investigations on age hardening, compounds of each of the  $T$  phases

Table 1. Analysis of *T* phase alloys

	Wt. % Mg	Wt. % Al	Wt. % third element	Remarks
Mg <sub>32</sub> (Al, Ag) <sub>49</sub> 6 : 1	28.1	43.5	28.4 (Ag)	Faint trace of second phase
Mg <sub>4</sub> CuAl <sub>6</sub>	30.3	50.0	19.7 (Cu)	Not quite single- phase
Mg <sub>4</sub> CuAl <sub>5</sub>	33.5	45.9	20.6 (Cu)	Single-phase
Mg <sub>32</sub> (Al, Cu) <sub>49</sub> 6 : 1	33.7	47.9	18.4 (Cu)	Single-phase
Mg <sub>32</sub> (Al, Zn) <sub>49</sub>	24.5	18.5	57.0 (Zn)	Not single-phase

mentioned above have been prepared and the present note reports the X-ray data obtained.

The compounds were prepared by melting, casting and then annealing a crushed portion of the alloy in evacuated Pyrex tubes at 460°C for several days and then slowly cooling. X-ray photographs were taken with an 11.46 cm diameter Guinier focusing camera with monochromatic  $K\alpha_1$  radiation and the relative intensities were obtained by microphotometry of the films.

For the Al-Mg-Ag *T* phase, after it had been found that a composition made to the Mg<sub>4</sub>AgAl<sub>6</sub> formula was not single-phase, a composition was made close to the analysis found by Wheeler *et al.*, who used microprobe analysis on a single-phase constituent. The actual analysis is given in Table 1. The composition corresponds closely to Mg<sub>32</sub>(Al, Ag)<sub>49</sub> with Al:Ag=6:1. The X-ray pattern, with the exception of one weak line, was able to be indexed as body centred cubic with  $a_0 = 14.52 \pm 0.01 \text{ \AA}$ .

In the Al-Mg-Cu system, compositions were made corresponding to Mg<sub>4</sub>CuAl<sub>6</sub>, Mg<sub>4</sub>CuAl<sub>5</sub> and Mg<sub>32</sub>(Al,Cu)<sub>49</sub> with Al:Cu=6:1. X-ray patterns showed that Mg<sub>4</sub>CuAl<sub>6</sub> was not quite single-phase but the other two compositions were. The pattern of Mg<sub>32</sub>(Al,Cu)<sub>49</sub> with  $a_0 = 14.35 \pm 0.01 \text{ \AA}$  is given in Table 2.

For comparison with the above two patterns, data for Mg<sub>32</sub>(Al,Zn)<sub>49</sub> are also given. This specimen was not entirely single phase and only the lines from the *T* phase are shown. The lattice parameter is  $14.22 \pm 0.01 \text{ \AA}$ .

Table 2. X-ray powder data of *T* phases

Mg <sub>32</sub> (Al, Ag) <sub>49</sub> 6 : 1		Mg <sub>32</sub> (Al, Cu) <sub>49</sub> 6 : 1		Mg <sub>32</sub> (Al, Zn) <sub>49</sub>		$h^2 + k^2 + l^2$
<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>	
10.25	40	10.22	30	10.08	90	2
5.95	20	5.89	10	5.80	45	6
5.15	4	5.10	2	5.03	16	8
4.60	4	4.55	4	4.49	35	10
				4.11	6	12
3.88	35	3.84	14	3.80	55	14
3.63	6	3.60	2	3.56	6	16
3.43	6	3.39	2	3.36	10	18
3.25	4	3.22	2	3.17	10	20
		3.06	2			22
2.849	4	2.818	6	2.789	6	26
2.653	4	2.623	4	2.597	6	30
2.569	2	2.540	2	2.519	2	32
2.492	100	2.466	100	2.440	100	34
2.423	35	2.388	35	2.374	30	36
2.356	95	2.331	100	2.307	100	38
2.296	2			2.248	6	40
2.239	2			2.192	2	42
2.186	2			2.142	4	44
2.141	50	2.117	25	2.095	70	46
2.053	55	2.030	40	2.012	85	50
2.013	25	1.991	12	1.976	18	52

Table 2 (cont.)

Mg <sub>32</sub> (Al, Ag) <sub>49</sub> 6 : 1		Mg <sub>32</sub> (Al, Cu) <sub>49</sub> 6 : 1		Mg <sub>32</sub> (Al, Zn) <sub>49</sub>		$h^2 + k^2 + l^2$
<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>	<i>d</i>	<i>I</i>	
1.977	10	1.953	6	1.937	20	54
		1.918	2	1.902	2	56
1.908	2	1.886	2	1.869	2	58
1.845	8	1.824	6	1.807	10	62
1.788	6	1.768	4	1.752	8	66
1.687	2	1.668	2	1.654	<2	74
		1.605	<2			80
1.566	4	1.548	2	1.535	2	86
1.546	2	1.531	2	1.517	2	88
1.530	4	1.514	2	1.499	4	90
1.497	2	1.481	2	1.464	2	94
1.466	30	1.450	18	1.437	25	98
1.452	8	1.436	4	1.422	8	100
1.423	2	1.408	<2	1.395	2	104
1.410	8	1.395	6	1.382	6	106
1.397	4	1.382	2	1.368	4	108
1.384	20	1.369	12	1.356	18	110
1.360	4	1.345	2	1.332	4	114
1.348	6	1.334	2	1.321	4	116
1.337	4	1.322	2	1.309	4	118
1.315	10	1.299	4	1.287	8	122
1.292	4	1.278	2	1.267	4	126
1.273	2					130
1.254	2	1.240	2			134
1.244	8	1.231	6	1.219	16	136
1.235	2	1.222	2	1.211	2	138
		1.213	<2			140
1.217	2	1.205	<2			142
1.210	4	1.197	<2	1.184	4	144
1.202	2					146
1.193	2					148
1.185	2	1.172	2			150
1.178	4	1.164	2	1.154	4	152
1.170	2					154
1.127	6	1.114	2	1.103	6	166
1.114	6	1.100	4	1.090	6	170
1.106	2	1.094	2	1.084	2	172
1.100	4	1.088	2	1.078	4	174
		$a_0 = 14.52$ $\pm 0.01 \text{ \AA}$		$a_0 = 14.35$ $\pm 0.01 \text{ \AA}$		$a_0 = 14.22$ $\pm 0.01 \text{ \AA}$

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## References

- BERGMAN, G., WAUGH, J. T. L. & PAULING, L. (1957). *Acta Cryst.* **10**, 254.  
 LAVES, F., LÖHBERG, K. & WITTE, H. (1935). *Metallwirtschaft*, **14**, 793.  
 NISHIMURA, H. (1937). *Mem. Coll. Eng. Kyoto Imperial University*, **10**, 18.  
 WHEELER, M. J., BLANKENBURGS, G. & STADDON, R. W. (1965). *Nature, Lond.* **207**, 746.