Short Communications

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Order in the ζ′ phase of the silver-gallium alloys.

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The ζ′ phase of the system Ag–Ga, which occurs around 75 at.% silver, is isomorphous with the ζ phase of the system Ag–Zn, which occurs around 50 at.% silver. A ternary single-phase region exists between the two binary phases. Edmunds & Qurashi (1951) determined the crystal structure of the AgZn ζ phase to be partially ordered and to belong to space group $C\bar{3}$. Crystallographic aspects of the relation between the AgZn ζ phase and the ordered body-centred cubic β′ phase from which it is derived have been examined by Kitchingman (1962) who showed that the order of the ζ phase is closely related to that of the β′ phase. No body-centred cubic phase exists in the Ag–Ga system, and in view of this and the composition difference of the ζ Ag–Zn and ζ′ AgGa alloys, the ordering of the ζ′ AgGa structure has been determined.

The AgGa alloy investigated contained 72 at.% silver. The lattice parameters at 20 °C determined from powder photographs with Cu $K\alpha$ radiation were:

$$a = 7{\cdot}7677 \pm 0{\cdot}0002,\ c = 2{\cdot}8778 \pm 0{\cdot}0001\ \text{Å}.$$

Intensity measurements of 33 reflexions were obtained from a flat powder sample with a Phillips X-ray diffractometer and filtered Cu $K\alpha$ radiation. Structure factors derived from line intensities were compared with those calculated assuming a random distribution of atoms in the unit cell, using the atomic coordinates of the ζ AgZn structure given by Edmunds & Qurashi. Since the residual index R for the observed and calculated structure factors was 0·13 over all the observed reflexions the structure was refined. Order parameters were introduced and refined together with the atomic parameters using the modified least-squares method of Qurashi (1949). The refinement showed that the atomic coordinates of the AgZn ζ phase could be used for the AgGa ζ′ phase without any correction. The order parameters indicated that the atomic position at the origin (0, 0, 0) is occupied exclusively by gallium atoms whilst the remaining gallium atoms and silver atoms occupy the two positions $(\frac{1}{3}, \frac{2}{3}, \frac{1}{4})$ and $(\frac{1}{3}, \frac{2}{3}, \frac{3}{4})$. The remaining silver atoms occupy the six positions derived by symmetry operations about the position (0·350, 0·032, 0·750). Table 1 shows the agreement between the observed and calculated structure factors using the refined parameters, the residual index R being 0·059 over all the observed reflexions.

Table 1. *The observed and calculated structure factors*

HKL	F_o	F_c	*HKL*	F_o	F_c
101	59	53	312	90	81
210	85	81	600	113	117
111	241	245	511	103	101
300	260	250	431	80	76
201	119	114	412 }	77	83
211	105	96	610 }		
221	194	200	521	124	119
320	56	51	530 }		
002	72	65	700 }	170	177
321	172	168	332 }		
411	205	205	422	98	102
330	156	144	620	61	70
420	106	92	441 }	80	97
212	56	64	203 }		
501	122	126	531 }	158	163
510 }	221	228	701 }		
302 }					

Thus the AgGa ζ′ phase and the AgZn ζ phase exhibit similar partial order as far as is compatible with the composition. The major difference is that each atom at the origin in the AgGa ζ′ phase is associated with at least six and possibly more unlike nearest neighbours compared with practically equal numbers of like and unlike nearest neighbours in the AgZn ζ phase.

References

Edmunds, I. G. & Qurashi, M. M. (1951). *Acta Cryst.* **4**, 417.

Kitchingman, W. J. (1962). *Acta Metallurg.* **10**, 799.

Qurashi, M. M. (1949). *Acta Cryst.* **2**, 404.