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The structure of β(AlCrSi).

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Mondolfo (1943) has reported the existence of two aluminium-rich ternary compounds in the Al–Cr–Si system, that with the higher silicon content (designated β) being thought to be monoclinic with a possible formula $CrSi_2Al_4$. Needle-shaped crystals of β(AlCrSi) with hexagonal cross-section, kindly supplied by Pratt & Raynor (1951), have an analysed composition of 32·2 atomic % Cr, 53·5 atomic % Si and (by difference) 14·3 atomic % Al, which is markedly different from the formula suggested by Mondolfo.

The crystallographic data obtained from single crystals are as follows:

Laue symmetry:	6/*mmm*.
Unit cell:	Hexagonal, $a_0 = 4{\cdot}49$, $c_0 = 6{\cdot}36$ Å.
Systematic absences:	h and k even with $l \neq 3n$ (n integral).
Space group:	D_6^4–$P6_22$ (or the enantiomorphous D_6^5–$P6_42$).
Density:	4·82±0·05 g.cm.$^{-3}$, giving 9·1±0·1 atoms, i.e. 3 'molecules' of Cr(Si, Al)$_2$, per unit cell.

More accurate cell dimensions have been determined from a powder photograph taken in a 19 cm. diameter camera with Cu $K\alpha$ radiation ($\lambda = 1{\cdot}5418$ Å) monochromatized by reflexion from a plane LiF crystal. Since there are insufficient strong high-angle reflexions for the use of extrapolation methods, c_0 has been estimated from fourteen determinations of δ_c, and a_0 from six determinations of δ_a, where

$$\delta_c = \sin^2\theta_2 - \sin^2\theta_1 = (\lambda^2/4c_0^2)(l_2^2 - l_1^2)\,,$$

θ_2 and θ_1 being the Bragg angles of the $(hk.l_2)$ and $(hk.l_1)$ reflexions, respectively, and

$$\delta_a = \sin^2\theta_4 - \sin^2\theta_3 = (\lambda^2/3a_0^2)\{(h_4^2+h_4k_4+k_4^2)-(h_3^2+h_3k_3+k_3^2)\}\,,$$

θ_4 and θ_3 applying to the $(h_4k_4.l)$ and $(h_3k_3.l)$ reflexions.

The lattice parameters estimated in this way are

$$a_0 = 4{\cdot}496 \pm 0{\cdot}002,\quad c_0 = 6{\cdot}377 \pm 0{\cdot}003 \text{ Å}\,.$$

The structure of the sample examined is found to be identical with that of the binary compound $CrSi_2$ (Borén, 1933) with aluminium replacing silicon to the extent of about one atom in five, viz.

$$3\,\mathrm{Cr}\ \text{in}\ 3d\ (\tfrac{1}{2}, 0, \tfrac{1}{2})\,,$$
$$6\,(\mathrm{Si, Al})\ \text{in}\ 6j\ (x, 2x, \tfrac{1}{2})\ \text{with}\ x = \tfrac{1}{6}$$

(see *International Tables*, 1952).

To account for the systematically absent reflexions, the x parameter of the (Si, Al) atoms must be exactly $\frac{1}{6}$, and a careful check has been made to establish that the absences are truly systematic. Chemical analyses, given by Pratt & Raynor (1951), of other samples of β(AlCrSi) suggest that, in addition to replacing silicon, aluminium atoms may also replace chromium, since the chromium content may be as low as 26·1 atomic %. β(AlCrSi) is not therefore a ternary compound, but merely a solid solution of aluminium in $CrSi_2$.

The formation of this compound in the aluminium-rich matrix is a precipitation effect, since it is reported (Pratt & Raynor) that there is no trace of its presence in alloys annealed at 550° C. for 21 days. Moreover, the occurrence of $CrSi_2$ in aluminium-rich alloys means that the structure must be of a high stability, which is probably due to an appreciable electrochemical factor. It is known that compound formation does tend to take place between solute atoms if they differ in size from the solvent atoms to an appreciable, though not too great, extent, and if the compound is reasonably stable (e.g. the formation of Mg_2Si in certain duralumin alloys (Hanson & Gayler, 1921)).

It is also of interest to note that the structure of $CrSi_2$ consists of successive close-packed sheets of atoms lying parallel to {0001}. With $a_0 = 4{\cdot}431 \pm 0{\cdot}005$ Å for $CrSi_2$ (Borén, 1933, converted from kX. units) the expansion in the {0001} plane of the lattice of the β(AlCrSi) sample examined, due to solution of 14·3 atomic % aluminium, is 1·47±0·16%. If the expansion were to continue at the same rate to 100% aluminium, the {0001} sheets would be close-packed with interatomic distances of 2·82±0·03 Å, which is very close to the interatomic distances in the {111} planes of the aluminium matrix (2·86 Å). It seems very likely, therefore, that the close-packed {0001} planes of $CrSi_2$ may grow out of the similarly close-packed {111} planes of the aluminium matrix.

Full details of this work are available in a Ph.D. dissertation (Robinson, 1951). The work was carried out whilst the author was in receipt of a grant from the Ministry of Supply (Basic Properties of Metals Committee).

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