The Crystal Structures of Y_3Al_2 and YAl

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The existence of phases in the yttrium-aluminium system of the compositions Y_3Al_2 and YAl was recently reported by Lundin and Klodt [1]. The crystal structures of the two compounds have now been determined from X-ray powder patterns.

The alloys were prepared by arc-melting the pure metals (yttrium 99.9 % and aluminium 99.99 %) in an argon atmosphere. The loss of weight of the sample during the arc-melting, was less than 1 % of the aluminium content. The samples were heat-treated at 600°C for 1 month in sealed tubes and quenched in water to room temperature. Guinier powder photograms of the alloys were taken using Cu$K\alpha_1$ radiation with potassium chloride added to the specimens as an internal standard.

The lines of the Y_3Al_2 pattern could be indexed with a tetragonal unit cell with

$a = 8.239 \pm 0.003$ Å, $c = 7.648 \pm 0.004$ Å, $c/a = 0.928$.

A unit cell content of 4 formula units of Y_3Al_2 gives a calculated density of 4.10 which is in agreement with the observed density of 4.06.

The phase is isomorphous with Zr_3Al_2 [2] and Hf_3Al_2 [3]. These phases both have the c/a ratio 0.918, and therefore the parameter values from these phases were tentatively adopted for the calculation of the line intensities of the powder pattern of Y_3Al_2. With the space-group $P4_2/mnm$ (No. 136) and the atoms in the following positions

8Al in 8(*j*)	with $x = 0.125$ and $z = 0.21$
4Y in 4(*f*)	with $z = 0.34$
4Y in 4(*g*)	with $x = 0.20$
4Y in 4(*d*)	

a good agreement between observed and calculated intensities for Y_3Al_2 was obtained.

The phase YAl was found to have an orthorhombic unit cell with:

$a = 3.884 \pm 0.002$ Å,
$b = 11.522 \pm 0.004$ Å,
$c = 4.385 \pm 0.002$ Å.

With 4 formula units of YAl in the cell the calculated density is 3.92 as compared with an observed value of 3.98.

The powder pattern showed YAl to be of the CrB-type and isomorphous with HfAl [4] and ThAl [5]. Starting with the parameter values reported for the latter phases, changing them slightly for geometrical reasons, it was possible to obtain a satisfactory agreement between calculated and observed intensities for the powder lines of YAl.

The following atomic arrangement of YAl was thus arrived at:

Space-group *Cmcm* (No. 63),

4Y in 4(*c*)	with $y = 0.43$
4Al in 4(*c*)	with $y = 0.15$

The accuracy of the parameter values of the two compounds is moderate, and refinement of the structures would require single-crystal data.

Further work on the crystal chemistry of the yttrium-aluminium system is in progress.

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