## Acta Cryst. (1960). 13, 743

## The structure of NbZn<sub>3</sub>. By C. L. VOLD, U. S. Naval Research Laboratory, Washington 25, D. C., U. S. A.

(Received 5 February 1960)

Table 1. Observed and calculated intensities for NbZn,

A study of the Nb-Zn system has been initiated in this laboratory to assist in understanding the high temperature oxidation resistance of zinc coated niobium. Preliminary studies have indicated the existence of at least three compounds. On the basis of weight gain data, the composition of the high zinc compound was estimated to be NbZn<sub>3</sub>. This composition was confirmed by a structure determination using the X-ray powder method and by chemical analysis.

The high zinc compound was prepared by reacting 6 mil. niobium foils with zinc vapor in evacuated  $(10^{-5}$  mm. Hg) and sealed silica capsules. The reaction was allowed to proceed at 870 °C. for 170 hr. (zinc pressure of 0.7 atmospheres), complete conversion to compound being obtained. This reaction product had a light grey color and showed a columnar grain structure. Both the appearance and the diffraction pattern were identical to those observed for the outer band of Nb–Zn diffusion couples.

The X-ray diffraction powder photographs were taken in a 114.6 mm. Debye-Sherrer camera, using Cu  $K\alpha$ radiation. All the lines could be indexed on a cubic unit cell with a lattice constant of 3.934 Å. There were no characteristic extinctions. Spatial considerations led immediately to the following trial structure, referred to space group  $Pm3m-O_{h}^{1}$ .

> 1 Nb in 1(a): 0, 0, 0. 3 Zn in 3(c):  $0, \frac{1}{2}, \frac{1}{2}; \frac{1}{2}, 0, \frac{1}{2}; \frac{1}{2}, \frac{1}{2}, 0.$

On the basis of this structure, the intensities were calculated and compared with those observed on the powder photograph (Table 1). Satisfactory agreement was obtained.

As this structure is of the Strukturbericht Type  $Ll_2$ , similar to AuCu<sub>3</sub>, the presence or absence of an order-

hkl	Ic	Io
100	<b>28</b>	w
110	<b>26</b>	w
111	1020	vs
200	480	8
210	15	vw
211	10	vw
220	310	m-s
300, 221	7	vvw
310	4	vvw
311	360	m-s
222	99	m
320	3	vvw
321	<b>5</b>	vvw
400	55	m
410, 322	<b>5</b>	vvw
411, 330	4	vvw
331	240	m-s
420	270	m-s
421	6	vvw
332	3	vvw
422	440	8

disorder transformation was investigated. X-ray examinations of samples quenched from 475 and 870  $^{\circ}$ C. showed no apparent reduction in the intensities of lines with mixed indices. It may therefore be concluded that no order-disorder transformation occurs within the temperature range considered, unless the solid state diffusion rates are sufficiently rapid to allow the transformation to occur during quenching. The latter possibility was not investigated.

The author is indebted to Dr R. A. Meussner for preparing the alloys and carrying out the quenching experiments.

## Acta Cryst. (1960). 13, 743

Some Laves phases of yttrium with transition elements.\* By B. J. BEAUDRY, J. F. HAEFLING and A. H. DAANE, Institute for Atomic Research and Department of Chemistry, Iowa State University, Ames, Iowa, U.S.A.

## (Received 3 February 1960)

In a study of phase diagrams of yttrium with metals of the first transition group, the cubic Laves phase (C15 type) has been found in the phase systems of yttrium with manganese, iron, cobalt and nickel. The peritectic nature of YNi<sub>2</sub> was shown by Beaudry & Daane (1960). The compounds YCo<sub>2</sub>, YFe<sub>2</sub>, and YMn<sub>2</sub> also appear to undergo peritectic decomposition on heating. Alloys containing 65.0, 66.7 and 68.0 at.% Mn, Fe, Co, and Ni with yttrium were prepared by co-melting the two metals in an arc melting furnace. To homogenize the arc-melted alloys, they were sealed in silica capsules under vacuo and annealed at 870 °C. for 125 hr., with the exception of the Y-Ni alloys which were annealed at 950 °C. for 100 hr. The alloys were cooled rapidly by dropping the silica capsules into water. The alloys were then ground to a powder in an agate mortar, sealed in Pyrex capillaries under vacuo and annealed at 400 °C. for three hr. to remove the effects of cold working. X-ray diffraction powder photographs were taken of the alloys using a Norelco camera of 114.6 mm. diameter and Cu K $\alpha$  radiation. Because the intensities of the reflections on the powder photographs of the different compounds are similar, only relative intensities for YNi<sub>2</sub> were calculated by means of the expression:

 $I \propto p |F_{hkl}|^2 (1 + \cos^2 2\theta) / (\sin^2 \theta \cos \theta)$ ,

<sup>\*</sup> Contribution No. 838. Work was performed in the Ames Laboratory of the U.S. Atomic Energy Commission.