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The structure of $NbZn_3$.

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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 $NbZn_3$. 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.

Table 1. *Observed and calculated intensities for* $NbZn_3$

hkl	I_c	I_o
100	28	*w*
110	26	*w*
111	1020	*vs*
200	480	*s*
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	5	*vvw*
400	55	*m*
410, 322	5	*vvw*
411, 330	4	*vvw*
331	240	*m–s*
420	270	*m–s*
421	6	*vvw*
332	3	*vvw*
422	440	*s*

As this structure is of the *Strukturbericht* Type $L1_2$, similar to $AuCu_3$, the presence or absence of an order–disorder transformation was investigated. X-ray examinations of samples quenched from 475 and 870 °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.

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Some Laves phases of yttrium with transition elements.*

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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_2 was shown by Beaudry & Daane (1960). The compounds YCo_2, YFe_2, and YMn_2 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_2 were calculated by means of the expression:

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

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* Contribution No. 838. Work was performed in the Ames Laboratory of the U.S. Atomic Energy Commission.

where p is the multiplicity factor, $F_{(hkl)}$ is the structure amplitude and the remaining term is twice the Lorentz and polarization factor. The scattering factors for both elements were obtained from the *Internationale Tabellen* (1935). Dispersion corrections from Dauben & Templeton (1955) were applied. The agreement between observed and calculated intensities for YNi_2 confirms the proposed structure for this compound. Some variation in the observed intensities due to the different dispersion of the Cu $K\alpha$ radiation by Ni, Co, Fe and Mn was noted, but still the agreement between the calculated intensities for YNi_2 and observed intensities for YCo_2, YFe_2 and YMn_2 leave little doubt that these compounds are all isostructural.

These cubic Laves phases belong to the space group O_h^7–$Fd3m$ with

$$8\,\mathrm{Y}\ \text{at: } 0, 0, 0;\ \tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{4},\ +\text{f.c.}$$

and

$$16M^*\ \text{at: } \tfrac{5}{8}, \tfrac{5}{8}, \tfrac{5}{8};\ \tfrac{7}{8}, \tfrac{7}{8}, \tfrac{5}{8};\ \circlearrowleft +\text{f.c.}$$

The lattice constants and interatomic distances for these four compounds are given in Table 1.

Table 1. *Lattice constants and interatomic distances*

Compound	a_0 (±0·002 Å)	Interatomic distances *A–A*	*B–B*	*A–B*
YNi_2	7·181 Å	3·109 Å	2·539 Å	2·977 Å
YCo_2*	7·216	3·125	2·551	2·991
YFe_2	7·357	3·186	2·601	3·050
YMn_2	7·680	3·325	2·715	3·184

* This lattice constant is in agreement with the value reported by Wernick & Geller (1960).

The compounds YMn_2, YFe_2 and YCo_2 have only a slight composition range, since only a decrease of 0·004 Å was noted between the 65·0 and 68·0 at.% M* alloys in these three cases. However, YNi_2 appears to have a composition range since its lattice constant in the 65·0 at.% Ni alloy was 7·183 ± 0·002 Å in the 68·0 at.% Ni alloy was 7·164 ± 0·001 Å. Atomic and molecular volume considerations indicate a composition range of 0·7 at.% in YNi_2.

References

Beaudry, B. J. & Daane, A. H. (1960). Y–Ni system. Submitted to *Trans. Amer. Inst. Min.* (*Metall*) *Engrs.*

Dauben, C. H. & Templeton, D. H. (1955). *Acta Cryst.* **8**, 841.

Internationale Tabellen zur Bestimmung von Kristallstrukturen (1935). Berlin: Borntraeger.

Wernick, J. H. & Geller, S. (1960). Rare-Earth Compounds with the $MgCu_2$ Structure. To be published in *Trans. Amer. Inst. Min.* (*Metall*) *Engrs.*

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* M = Ni, Co, Fe or Mn.

Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. The notes (in duplicate) should be sent to the General Secretary of the International Union of Crystallography (Dr D. W. Smits, Laboratory of Inorganic and Physical Chemistry, 10 *Bloemsingel, Groningen, The Netherlands).*

Pittsburgh Diffraction Conference

The annual Pittsburgh Diffraction Conference will be held November 9–11, 1960, at Mellon Institute, Pittsburgh, Pennsylvania, U. S. A. Sessions will be devoted to metals and alloys, instrumentation, structures, polymers and fibres, refractories, electron probes and electron diffraction. The evening meeting will be addressed by Professor I. Fankuchen of the Polytechnic Institute of Brooklyn. Further information can be obtained from L. F. Vassamillet, Mellon Institute, 4400 Fifth Avenue, Pittsburgh 13, Pennsylvania.