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INTERMETALLIC COMPOUNDS OF YTTRIUM
FINAL REPORT

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INTRODUCTION

The first objective of this investigation was to determine the phase diagram for the yttrium-cadmium binary system, and thus determine what intermetallic compounds occur in this system. The crystal structures of these compounds were to be studied and compared to those of other yttrium binary compounds in an attempt to learn something about the interatomic bonding in these materials.

The second objective of this investigation was to investigate the phase relations in the yttrium-cadmium-zinc alloy system in an attempt to determine the extent to which zinc atoms could be substituted for cadmium atoms and vice versa. This would provide information on the effect of changes in size and perhaps bonding type on alloy formation.

Finally, it was hoped that an investigation of the relationship between the crystal structure of the yttrium-cadmium intermetallic compounds and their mechanical properties could be begun.

RESULTS AND DISCUSSION

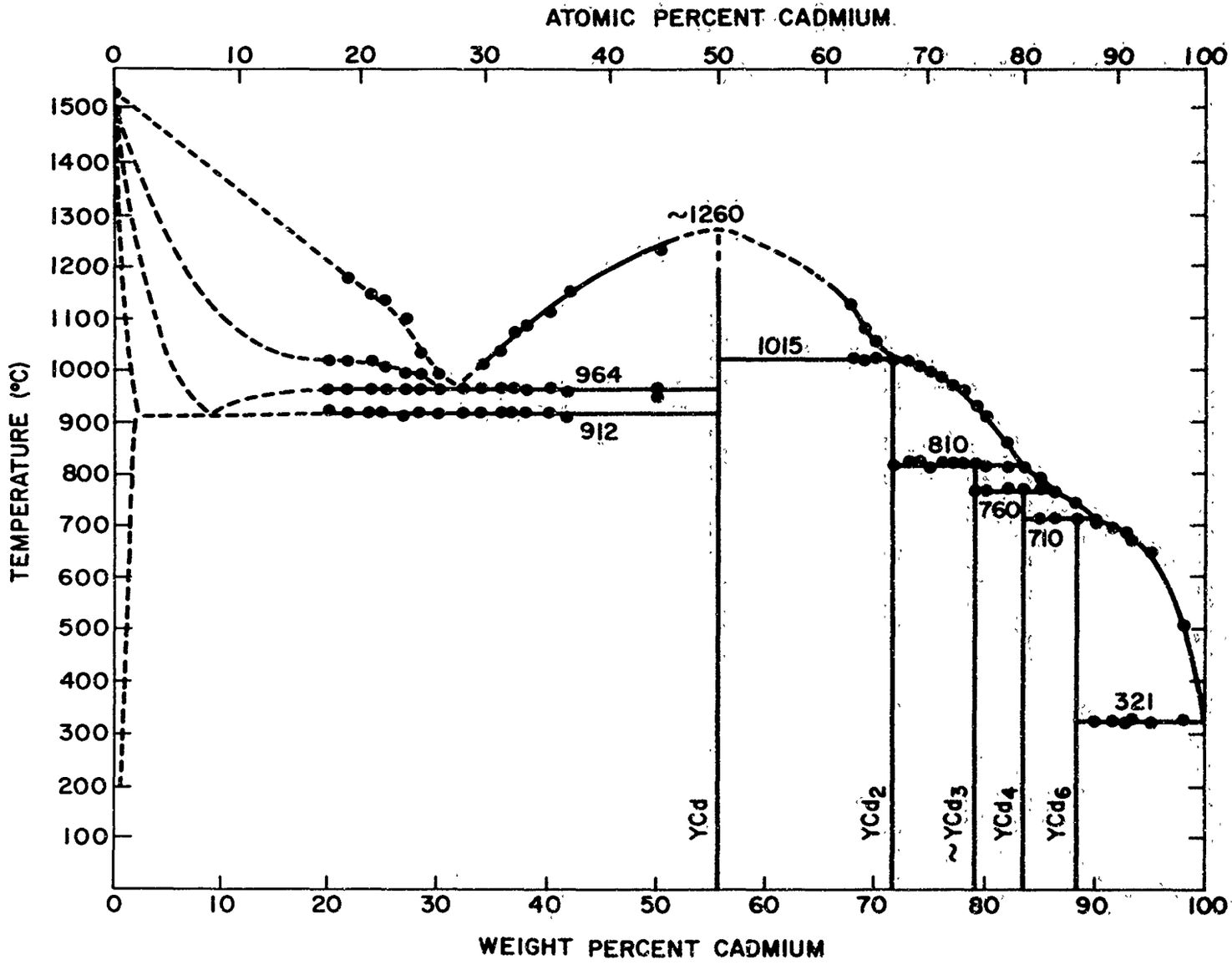
The principal results of this work are as follows:

1. The Y-Cd phase diagram was determined
2. Crystallographic data were obtained for these Y-Cd intermediate phases:
   a. YCd_2
   b. YCd_3
   c. YCd_4
   d. YCd_6
3. The YCd_3-Zn pseudo-binary phase diagram was determined
4. Crystallographic data were obtained for these Y-Cd-Zn intermediate phases:
   a. $Y_3(Cd_9Zn_2)$
   b. $Y_3(Cd_4Zn_7)$
   c. $\sim Y_2(CdZn_{14})$

The Y-Cd phase diagram, determined from differential thermal analysis, metallographic, and x-ray diffraction studies, is shown in figure 1. The intermediate phases which occur in this binary system are YCd, YCd_2, YCd_3, YCd_4, and YCd_6. All appear to be line compounds, and all except YCd decompose peritectically rather than melt congruently. Part of the phase diagram, in the high yttrium region and near the compound YCd, is still undetermined because of the high melting temperatures. However, from the data obtained and the results of other investigators, it was ascertained that cadmium stabilizes the high temperature form of yttrium, and the thermal arrests have been interpreted with this in mind.

The phase diagram is at variance with the results of Bruzzone & Ruggiero (1963) who state that YCd, along with YCd_2 and YCd_3, melt below 1100°C. YCd is estimated to melt at about 1260°C.

Figure 1. The yttrium-cadmium phase diagram


ATOMIC PERCENT CADMIUM
0
10
20
30
40
50
60
70
80
90
100
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
TEMPERATURE (°C)
~1260
1015
964
912
810
760
710
321
YCd
YCd2
~YCd3
YCd4
YCd6
WEIGHT PERCENT CADMIUM

The intermetallic compounds in this system have the following structures: YCd – CsCl type; YCd_2 – AlB_2 type; YCd_3 – $PrMg_3$ type, all of which were previously determined by other investigators, but verified in this investigation. In the case of hexagonal YCd_2, the z positional parameter for the Cd atoms is variable in the crystallographic sense, but apparently was not previously determined. This parameter was determined from single crystal x-ray intensity measurements to be z = 0.4783. YCd_4 was found in this investigation to be cubic with a = 21.492 Å, and appears to have a structure which is based upon an ordered arrangement of Y and Cd atoms in body-centered cubic subcells. YCd_6 was found in this investigation to be either orthorhombic or tetragonal, body-centered with $a \approx b \approx c \approx 15.48$ Å. This is in disagreement with Johnson, Schablaske, Tani & Anderson (1964), who state that YCd_6 is primitive cubic. The results of these investigators were based only upon powder patterns and appear to be incorrect in view of the results of the single crystal x-ray studies carried out in the present investigation. YCd_6 appears to have a structure quite similar to that of YCd_4. The determination of the crystal structures of YCd_4 and YCd_6 are, however, not yet complete. The crystallographic data are summarized in Table I.

The 0-20 w/o Zn portion of the phase diagram for the YCd_3-Zn pseudo-binary section is shown in figure 2. An intermediate phase, whose composition was determined by density measurements and neutron activation analysis to be $Y_3(Cd_9Zn_2)$, occurs in this range. This line compound, which decomposes eritectically, is hexagonal with a = 15.103, c = 14.985 Å.

The phase diagram for the rest of the YCd_3-Zn pseudo-binary section is shown in figure 3. The results shown there are viewed as somewhat tentative since the reactions cannot be defined with confidence until more ternary alloys are studied.

Table I
Crystallographic data for Y-Cd Intermetallic Compounds

YCd

Lattice parameter: a = 3.707 Å (also a = 3.712 Å)

Space group: Pm3m

Structure: CsCl-type — Y atoms at (000); Cd atoms at $(\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2})$

No studies of this compound in the present investigation. Above results were obtained by Bruzzone & Ruggiero (1963) and Laube & Nowotny (1963).

YCd_2

Lattice parameters: a = 4.882 ± 1, c = 3.501 ± 3 Å (also a = 4.879, c = 3.500 Å)

Space group: $P\bar{3}m1$

Structure: CdI_2-type — Y atoms at (000); Cd atoms at $(\frac{1}{3}\ \frac{2}{3}\ z)$, $(\frac{2}{3}\ \frac{1}{3}\ \bar{z})$
z = 0.4783 ± 14.

Lattice parameters in parentheses obtained by Bruzzone & Ruggiero (1963)

YCd_3

Lattice parameter: a = 7.412 ± 1 Å (also a = 7.174 Å)

Space group: Fm3m

Structure: $PrMg_3$ or BiF_3-type — Y atoms at (000), etc; Cd atoms at $(\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2})$, etc. and $(\frac{1}{4}\ \frac{1}{4}\ \frac{1}{4})$, $(\frac{3}{4}\ \frac{3}{4}\ \frac{3}{4})$, etc.

Lattice parameter in parentheses obtained by Bruzzone & Ruggiero (1963)

YCd_4

Lattice parameter: a = 21.492 ± 4 Å

Space group: F432 or Fm3m

Density: d_m = 7.21 gm/cm^3; d_x = 7.19 gm/cm^3 (432 atoms/unit cell)

Structure: Not completely determined. Appears to be based upon an ordered arrangement of Y and Cd atoms in body-centered cubic subcells. 432 atoms/unit cell implies that the stoichiometry is Y_5Cd_{22}.

YCd_6

Lattice parameters: a = 15.479 ± 14, b = 15.481 ± 10, c = 15.46 Å

Space group: I222, $I2_12_12_1$, Imm2, or Immm (or tetragonal equivalents)

Structure: Not completely determined. Related to YCd_4.

Johnson, Schablaske, Tani & Anderson (1964) reported that YCd_6 is primitive cubic with a = 15.479 Å.

Figure 2. 0-20 w/o Zn portion of the phase diagram for the YCd_3-Zn pseudo-binary section of the yttrium-cadmium-zinc alloy system.

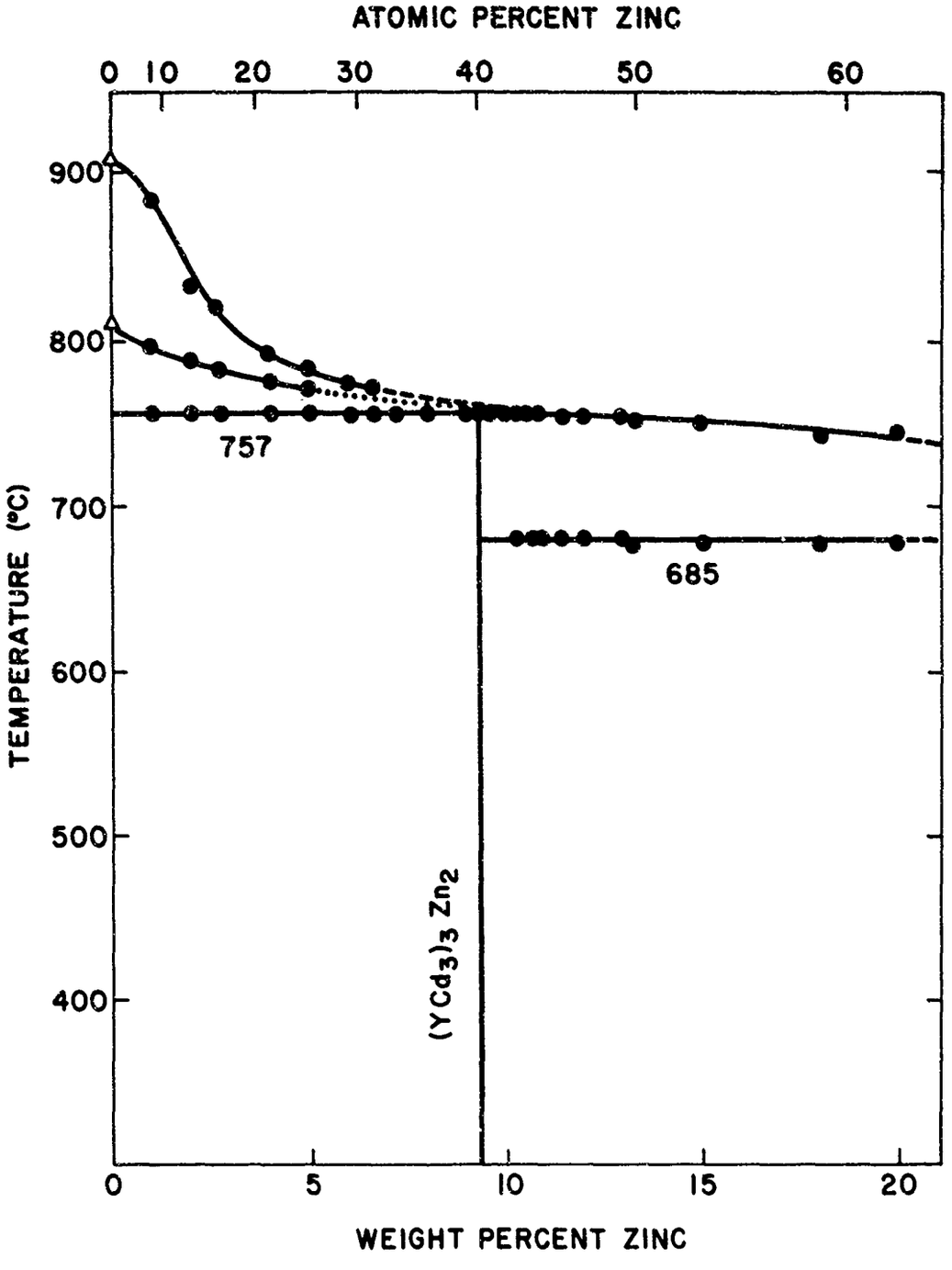
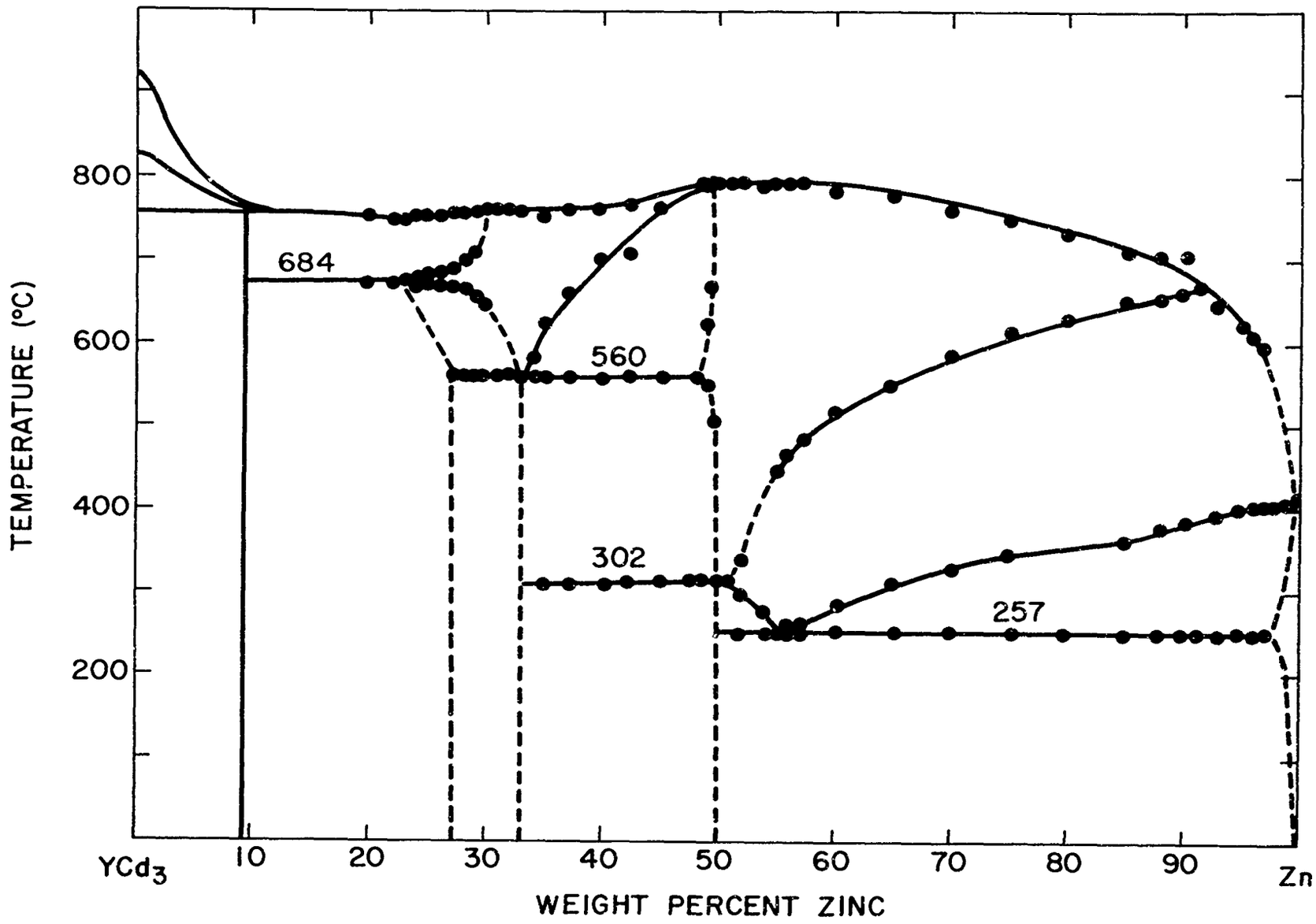

ATOMIC PERCENT ZINC
0 10 20 30 40 50 60
900
800
700
600
500
400
TEMPERATURE (°C)
757
685
$(YCd_3)_3 Zn_2$
0 5 10 15 20
WEIGHT PERCENT ZINC

Figure 3. The phase diagram for the YCd_3-Zn pseudo-binary section of the yttrium-cadmium-zinc alloy system.


TEMPERATURE (°C)
800
600
400
200
684
560
302
257
YCd3
10
20
30
40
50
60
70
80
90
Zn
WEIGHT PERCENT ZINC

Two additional ternary intermediate phases were found to occur in the alloys on this section. These compounds do not have compositions which lie on the section. Their compositions were estimated from electron microprobe analyses, and several alloys near the estimated compositions were prepared. A single phase alloy was obtained at $Y_3(Cd_4Zn_7)$, and the alloy at $Y_2(CdZn_{14})$ was nearly one phase. $Y_3(Cd_4Zn_7)$ is orthorhombic with a = 14.477, b = 14.669, c = 25.507 Å and $\sim Y_2(CdZn_{14})$ is monoclinic with a = 10.234, b = 9.038, c = 6.822 Å, β = 99.4°. The crystallographic data for these compounds are summarized in Table II. The compounds $Y_3(Cd_4Zn_7)$ and $Y_3(Cd_9Zn_2)$ probably have crystal structures which are based upon the structure of Y_3Zn_{11} (Ryba, Sree Harsha & Somerfeldt, 1970), in which, at certain compositions, Cd atoms substitute in an ordered fashion for Zn atoms. Small distortions in the Y_3Zn_{11} structure result which change the symmetry. In view of this hypothesis, it seems unlikely that these intermediate phases exhibit any solid solubility in this ternary system. In addition, several other questions are raised: (1) are there other $Y_3(Cd, Zn)_{11}$ ternary phases; (2) does this ordered substitution of Cd atoms for Zn atoms occur for the structures of the other seven Y-Zn intermetallic compounds; and (3) if not, why is the Y_3Zn_{11} structure able to accommodate the substituted Cd atoms?

Table II
Crystallographic Data for Three Y-Cd-Zn
Ternary Intermetallic Compounds

$\underline{Y_3(Cd_9Zn_2)}$

Lattice parameters:	a = 15.103 ± 4, c = 14.985 ± 6 Å
Space group:	$P\bar{6}2c$, $P6_3mc$, or $P6_3/mmc$
Density:	d_m = 6.084 gm/cm^3; d_x = 6.081 gm/cm^3 (8 formula weights/unit cell)
Structure:	Not completely determined. Appears to be based upon an ordered substitution of Cd atoms for Zn atoms in the Y_3Zn_{11}-type structure.

$\underline{Y_3(Cd_4Zn_7)}$

Lattice parameters:	a = 14.477, b = 14.669 ± 8, c = 25.507 Å
Space group:	$Pn2_1a$ or Pnma
Structure:	Not completely determined. Probably related to $Y_3(Cd_9Zn_2)$.

$\sim\underline{Y_2(CdZn_{14})}$

Lattice parameters:	a = 10.234 ± 6, b = 9.038 ± 5, c = 6.822 ± 9 Å, β = 99.4°
Space group:	C2, Cm, or C2/m
Structure:	Not completely determined.

A study of the mechanical properties of the Y-Cd intermetallic compounds was begun, but time and some difficulties in sample preparation prevented a detailed study of these properties. Attempts to prepare sintered samples according to the technique developed by Michel & Ryba (1968) were unsuccessful. It appears that an exploratory study of sintering times and temperatures will be necessary before sound, homogeneous samples can be produced. A summary of the hardness and ductility characteristics of these compounds is given in Table III. As expected, compounds with high cadmium contents exhibit more ductility and are softer. The existence of some ductility in YCd_4 and YCd_6 is rather usual since rare earth intermetallic compounds are usually quite brittle.

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Johnson, Schablaske, Tani & Anderson (1964). Trans. AIME 230, 1485.

Laube & Nowotny (1963). Monatsh. Chem., Osterr. 94, 851.

Michel & Ryba (1968). J. Less-Common Metals 16, 74.

Ryba, Sree Harsha & Somerfeldt (1970). To be submitted to Acta Cryst.

Table III
Microhardness and Ductility Characteristics
for Y-Cd Intermetallic Compounds

Compound	Microhardness (kg/mm^2)	Ductility
YCd_2	146	Brittle
YCd_3	163*	Extremely Brittle
YCd_4	121	Very Slightly Ductile
YCd_6	99	Slightly Ductile, "Flaky"

* Extensive cracking observed.

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1. Elmendorf & Ryba (1968). A note on the structure of YCd_2. Acta Cryst. B24, 462.

2. Ryba, Kejriwal & Elmendorf (1969). The partial yttrium-cadmium phase diagram. J. Less-Common Metals 18, 419.

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4. Ryba & Hahn (1970). Ternary intermediate phases in the yttrium-cadmium-zinc system. (To be submitted to J. Less-Common Metals.)

THESES

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Hahn (1969). Partial determination of phase diagram for the YCd_3-Zn pseudo-binary section of the Y-Cd-Zn system. M.S. thesis in Metallurgy, The Pennsylvania State University.

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13. ABSTRACT

The first objective of this investigation was to determine the phase diagram for the yttrium-cadmium binary system, and thus determine what intermetallic compounds occur in this system. The crystal structures of these compounds were to be studied and compared to those of other yttrium binary compounds in an attempt to learn something about the interatomic bonding in these materials. The second objective of this investigation was to investigate the phase relations in the yttrium-cadmium-zinc alloy system in an attempt to determine the extent to which zinc atoms could be substituted for cadmium atoms and vice versa. This would provide information on the effect of changes in size and perhpas bonding type on alloy formation. Finally, it was hoped that an investigation of the relationship between the crystal structure of the yttrium-cadmium intermetallic compounds and their mechanical properties could be begun.

14. KEY WORDS

Alloying, Binary systems (materials), phase diagrams, intermetallics, crystal structure

Chemical bonds, Cadmium inorganic compounds, Cadmium alloys, Cadmium containing alloys,

Yttrium compounds, Yttrium alloys, Zinc alloys, Zinc containing alloys, Zinc inorganic compounds
Ternary systems

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