Crystal Structure and Some Properties of the Compound, Zr_3Al

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THE crystal structure of Zr_3Al , the compound richest in zirconium (91.03 pct Zr by weight) in the system Zr-Al, has been found to be ordered face-centered-cubic. This compound is of particular interest, since it is encountered as the precipitated phase in potentially useful zirconium-rich alloys. It forms peritectoidally from body-centered-cubic zirconium and Zr_2Al at about 975°C. The Zr-Al constitution diagram has been reported by McPherson and Hansen.¹

For the primary determination a 100 g ingot was prepared by arc-melting in a water-cooled copper crucible under purified argon. The raw materials were crystal-bar zirconium (a purity of better than 99.7 pct) and spectroscopically pure aluminum. The ingot was double melted, examined metallographically, and found to be quite uniform as shown in Fig. 1. The hardness of the as-cast button was VHN 390 to 445.

A 20 mil diam specimen was prepared from annealed (900°C) filings of Zr_3Al . The specimen was mounted in a 5 cm radius powder camera and an 8 hr exposure was taken using copper radiation with a nickel filter.

The structure of the compound Zr_3Al was found to be ordered face-centered-cubic of the Cu_3Au type, with an a_0 value of $4.372 \pm 0.003 \text{ \AA}$. Its calculated density is $5.976 \pm 0.013 \text{ g per cu cm}$. The relative intensities for the lines were calculated using the formula

$$I \propto \frac{1 + \cos^2 2\theta}{\sin^2 \theta \cos \theta} \cdot p \cdot /F^2/$$

where $\frac{1 + \cos^2 2\theta}{\sin^2 \theta \cos \theta}$ is the Lorentz polarization factor, p is the multiplicity factor, and F is the structure factor. The X-ray data are given in Table I.

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Fig. 1—Micrograph of as-cast Zr_3Al shows a fairly uniform structure. Bright field, etched in HNO_3 , HF, and glycerine. X100. Area reduced approximately 20 pct for reproduction.

Table I. X-Ray Data for Compound Zr_3Al

hkl	Calculated d	Observed d	Calculated Intensity	Observed Intensity
100	4.372	4.38	227	Medium
110	3.091	3.09	186	Medium
111	2.524	2.52	1543	Very strong
200	2.186	2.18	760	Strong
210	1.955	1.95	97	Weak
211	1.785	1.78	71	Weak
220	1.546	1.54	470	Strong
300,221	1.457	1.46	9 to 35	Weak
310	1.383	1.38	57	Weak
311	1.318	1.32	517	Strong
222	1.262	1.26	154	Medium to strong
320	1.212	1.22	38	Very weak
321	1.168	1.17	39	Weak
400	1.093	1.09	79	Medium
410,322	1.060	1.06	14 to 14	Very weak
411,330	1.030	1.03	13 to 7	Very weak
331	1.003	1.003	276	Medium to strong
420	0.9776	0.977	267	Medium to strong
421	0.9540	0.953	26	Very weak
332	0.9321	0.931	14	Very weak
422	0.8924	0.892	279	Strong
500,430	0.8744	0.873	4 to 15	Very very weak
510,431	0.8574	0.857	16 to 31	Very weak
511,333	0.8414	0.841	336 to 112	Strong
520,432	0.8119	0.812	45 to 45	Weak
521	0.7982	0.798	55	Weak

The compound has exhibited plasticity when present as particles in a matrix of α zirconium. During hot working at about 900°C, the compound has been found to deform plastically to the extent that some of the particles exhibit a length-to-width ratio greater than 4:1 as shown in Fig. 2. In answer to the discussion of ref. 1, McPherson and Hansen pointed out that the compound may be cold rolled and reduced as much as 33 pct.

Zr_3Al has also been found² under certain conditions to precipitate in lamellar form at grain boundaries of the α phase of hexagonal-close-packed zirconium.

Acknowledgment

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¹ D. J. McPherson and M. Hansen: *Trans. ASM* (1954) 46, p. 354.

² J. H. Keeler: *Trans. ASM* (1954) 46, p. 373.

Fig. 2—Micrograph of specimen shows elongated particles of Zr_3Al in a matrix of α zirconium. The specimen of 10 atomic pct Al in zirconium was hot rolled at 900°C and then annealed 1 hr at 850°C. Bright field, etched in HNO_3 , HF, and H_2O . X500. Area reduced approximately 20 pct for reproduction.