The Crystal Structure of V_3Co

by Pol Duwez

IN the course of an investigation of the V-Co system, two intermediate phases were found. One of these phases corresponds approximately to the stoichiometric composition VCo and is isomorphous with the sigma phase in the Fe-Cr system.¹ The second phase has the composition V_3Co ; its crystal structure is described in the present note.

The alloys were prepared by mixing the two metals in the powder form, pressing a small disk weighing about 5 g at 80,000 psi, and arc melting this disk on a water-cooled copper plate in an atmosphere of pure helium. The details of this technique have been described.² The vanadium powder was obtained from Westinghouse Electric Corp., Bloomfield, N. J. This powder is probably of very high purity, since when it is properly sintered or melted in the above-mentioned arc furnace, ductile specimens are obtained. The cobalt powder, from Charles Hardy, Inc., New York, contained 0.5 pct Ni, 0.1 pct Cr, and traces of Si and Fe.

After melting, the V_3Co samples were sealed in evacuated quartz tubes and homogenized for ten days at 800°C. Powder diffraction patterns were obtained with a 14.32 cm diam camera, using $K\alpha$ copper radiation. The patterns were readily indexed on the basis of a primitive cubic lattice with a parameter equal to 4.675 Å. The density, determined by the immersion method, was 6.71 g per cu cm; hence the number of molecules per unit cell is approximately 1.95; i.e., 2.

At this point, the possibility that the structure might be that of beta tungsten³ became apparent. The beta tungsten structure is described as follows:

Space group $O_h^3 - Pm\bar{3}n$

2 Co in (a) : 000; $\frac{1}{2}\frac{1}{2}\frac{1}{2}$

6 V in (c) : $\frac{1}{4}0\frac{1}{2}$; $\frac{1}{2}\frac{1}{4}0$; $0\frac{1}{2}\frac{1}{4}$; $\frac{3}{4}0\frac{1}{2}$;
 $\frac{1}{2}\frac{3}{4}0$; $0\frac{1}{2}\frac{3}{4}$

(hhl) reflection present only if $l = 2n$.

Assuming this structure to be the correct one, intensities were computed by means of the usual equation:

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

where F is the structure factor, θ the Bragg angle, and p the multiplicity factor. The observed and calculated values of $\sin \theta$ and the intensities are given in Table I. The agreement between the observed and the calculated $\sin \theta$ is good and there are no flagrant discrepancies between the calculated intensities and those estimated visually. The (hhl) reflections for which l is odd are not observed, as required by the space group. In addition, the (410), (430), and (531) reflections are missing as expected, because of the special (a) and (c) positions in O_h^3 . However, six reflections—(110), (220), (310),

(411), (422), and (510)—which have very weak computed intensities were not observed. For these reflections, the structure factor is proportional to the difference between the scattering factors of the two atoms in the structure. Since the scattering factors of vanadium and cobalt are not very different, these reflections are weak. However, by using $K\alpha$ chromium radiation, whose wavelength is just above the absorption edge of vanadium, the effective scattering factor of vanadium may be decreased by one or two units; consequently the difference between the cobalt and vanadium scattering factors is increased. It was, indeed, found that in a powder pattern taken with chromium $K\alpha$ radiation, the three reflections (110), (220), and (310) were actually present. The three other reflections (411), (422), and (510), with spacings smaller than half the wavelength of chromium $K\alpha$, were obviously not obtainable with chromium radiation.

All the experimental results appear to confirm the beta tungsten structure for V_3Co . In this structure,

Table I. Diffraction Data for V_3Co

hkl	d , Å	$\sin^2 \theta$ (Observed)	$\sin^2 \theta$ (Computed)	Intensity (Observed)	Relative Intensity (Computed)
110*			0.0543		21
200	2.34	0.1079	0.1086	m	425
210	2.08	0.1366	0.1357	s	1000
211	1.90	0.1637	0.1628	s	880
220*			0.2171		3
310*			0.2714		6
222	1.349	0.3262	0.3257	vw	58
320	1.296	0.3534	0.3528	w	195
321	1.247	0.3818	0.3800	m	430
400	1.165	0.4369	0.4342	w	145
411-330			0.4885		2
420	1.044	0.5442	0.5428	w	130
421	1.019	0.5714	0.5699	vw	53
332	0.9962	0.5978	0.5971	w	125
422			0.6514		1
510-431			0.7056		3
520-432	0.8686	0.7864	0.7871	m	320
521	0.8535	0.8143	0.8142	m	290
440	0.8266	0.8683	0.8685	m	300

Quadratic form for copper $K\alpha_1$ radiation:

$$\sin^2 \theta = 0.02714 (h^2 + k^2 + l^2)$$

s = strong; m = medium; w = weak; vw = very weak.

* Reflection observed in a pattern obtained with chromium $K\alpha$ radiation.

each cobalt atom is surrounded by twelve vanadium atoms at 2.61 Å; each vanadium atom is surrounded by two vanadium atoms at 2.34 Å, four cobalt atoms at 2.61 Å, and eight vanadium atoms at 2.86 Å.

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