

High Temperature Modification of TiCr₂

by B. W. Levinger

THE system Ti-Cr has been studied by several investigators.¹⁻⁴ Though titanium and chromium are completely miscible at high temperatures, an intermediate phase of the approximate atomic proportions TiCr₂ has been identified at various compositions between 60 and 68 wt pct Cr. The structure of this phase was established as the cubic C15 (MgCu₂) type with 24 atoms per unit cell and a lattice parameter 6.929 kX.⁵

During a study of the ternary system, Ti-Mo-Cr,⁶ the existence of a high temperature modification of the TiCr₂ phase was discovered. In a series of alloys annealed at 1300°C and containing from 60 to 70 wt pct Cr and 5 pct Mo, a new phase was present which did not correspond to either β solid solution or TiCr₂. By trial, the new phase was identified to be of the hexagonal C14 (MgZn₂) structure with 12 atoms per unit cell. Further work showed that the hexagonal structure was, in fact, also present in binary Ti-Cr alloys quenched from high temperatures.

To make the identification more certain, the intensities of the various reflections were calculated assuming a composition TiCr₂ and C14 structure. Table I lists reflection planes, interplanar distances, calculated intensities, and a comparison of these values with the lines of a binary Ti-Cr alloy (66 pct Cr) annealed for 20 min at 1385°C and water quenched. Since high angle lines were more diffuse, the correspondence between visually observed and calculated intensities was not as good at these angles.

Lattice parameters were computed to be $a = 4.922$ kX, $c = 7.945$, $c/a = 1.614$. The corresponding interatomic distances are: titanium to titanium distance, 3.00, kX, chromium to chromium distance, 2.43, kX, titanium to chromium distance, 2.88, kX. These compare to 3.00, 2.45, and 2.87 kX in the cubic phase, respectively.²

The atomic positions in the C14 structure are as follows:

Titanium $1/3, 2/3, z; 1/3, 2/3, 1/2-z;$
 $2/3, 1/3, z; 2/3, 1/3, (1/2-z);$

Chromium $0, 0, 0; 0, 0, 1/2;$
 $2x, x, 1/4; 2x, x, 3/4;$
 $x, 2x, 1/4; x, 2x, 3/4;$
 $x, x, 1/4; x, x, 3/4;$

The values of x and z were calculated for the alloy mentioned and found as follows: $z = 0.061, x = 0.165$. The values assumed in the intensity calculations were those for an ideal close-packed lattice or $z = 1/16, x = 1/6$.

Work in the Ti-Mo-Cr system indicates that γ_2 , the hexagonal modification of TiCr₂, is the stable phase above 1300°C, while γ_1 with the cubic structure is stable below 1000°C. X-ray examination of a number of alloys annealed at intermediate temperatures showed that the hexagonal and cubic phases can coexist. Alloys quenched from 1000°C and annealed at 1100° and 1200°C showed small

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Table I. Diffraction Data for TiCr₂ (γ_2 Phase)

hkl	d, Calculated* (kX)	d, Observed† (kX)	Intensity Observed‡	Relative Intensity Calculated§	Corresponding Data ² for γ_1	
					d (kX)	hkl
110	2.461	2.454	w	0.14	2.44	220
103	2.250	2.247	wm	0.36		
200	2.131	2.127	vft	0.05		
112	2.092	2.087	m	0.57	2.08	311
201	2.058	2.056	m	0.54		
004	1.986	1.985	w	0.13	1.99	222
202	1.878	1.876	w	0.13		
104	1.800	1.798	vw	0.07	1.73	400
203	1.660	1.657	ft	0.04		
210	1.611	1.610	vft	0.01	1.59	331
300	1.421	1.419	vft	0.02	1.411	422
213	1.376	1.377	wm	0.15		
302	1.338	1.337	wm	0.14	1.333	511
006	1.317	1.323	vft	0.02		
205	1.274	1.272	wm	0.23		
214	1.251	1.251	vw	0.06		
220	1.230	1.229	wm	0.21	1.223	440
206	1.125	1.124	w	0.17	1.167	531
107	1.097	1.095	vft	0.04	1.094	620
313	1.079	1.078	w	0.17		
401	1.056	1.055	vw	0.17	1.057	533
224	1.046	1.045	w	0.27	1.045	622
402	1.029	1.029	vft	0.06		
314	1.016	1.015	ft	0.08		
207	1.002	1.001	vft	0.07	0.9976	444
108	0.9672	0.9686	ft	0.10	0.9708	711
410	0.9301			0.06	0.9255	642
217	0.9279	0.9285	ft	0.08		
323	0.9173	0.9171	vw	0.21		
412	0.9056			0.19	0.9021	731
226	0.9014	0.9052	wm	0.21		
405	0.8850	0.8851	w	0.37	0.8662	800
218	0.8454	0.8453	w	0.34		
406	0.8302	0.8306	vw	0.37		
317	0.8187	0.8186	ft	0.15	0.8168	822
308	0.8139	0.8138	ft	0.13		
332	0.8033	0.8035	w	0.53		
421	0.8014	0.8013	wm	1.00	0.8003	555
0010	0.7945	0.7950	vft	0.11	0.7946	662
422	0.7894	0.7894	vw	0.48		
504	0.7834	0.7837	ft	0.20		
407	0.7769	0.7769	vft	0.61	0.7746	840

* d observed from an alloy containing 66 pct Cr-34 pct Ti water quenched from 1385°C.

† d calculated from lattice parameters: $a = 4.922$ kX, $c = 7.945$. These lattice parameters were obtained by the method of least squares from eight lines of the above pattern.

‡ Observed Intensity: m, medium; wm, weak medium; w, weak; vw, very weak; ft, faint; vft, very faint. In a number of cases, lines were diffuse and it was felt that they represented a pair of lines. This is indicated by bracketing.

§ Relative Calculated Intensity: The values of relative intensity for planes from (110) to (220) are due to Wallbaum.⁶ Actually they represent corresponding values for the isomorphous phase, TiMn₂; calculation of a number of lines at higher angles showed that the two values correspond within a few percentage points.

amounts of γ_2 at the higher temperature. A considerable amount of γ_2 seemed present, however, in cast alloys annealed at 1100°C. It further appears that there is a small but definite solubility range for both phases in the ternary system.

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