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The crystal structure of $\text{Ti}(\text{Pt}_{0.89}\text{Ni}_{0.11})_3$. By ASHOK K. SINHA,* *Department of Metallurgy, University of Illinois, Urbana, Illinois 61801, U.S.A.*

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$\text{Ti}(\text{Pt}_{0.89}\text{Ni}_{0.11})$ crystallizes in the trigonal system with $a = 5.491 \pm 0.003$, $c = 15.67 \pm 0.01$ Å; space group $P\bar{3}m1$ with 28 atoms per unit cell. The structure may be derived from triangularly ordered, close packed AB_3 layers by stacking them in the sequence $\dot{a}cab\dot{c}ab\dot{c}$.

In his investigation of the quasi-binary system $\text{TiPt}_3\text{-TiNi}_3$, van Vucht (1966) reported a hexagonal intermediate phase of undetermined structure at the composition $\text{Ti}(\text{Pt}_{0.89}\text{Ni}_{0.11})_3$. The present investigation was undertaken to determine this crystal structure.

The alloy $\text{Ti}(\text{Pt}_{0.89}\text{Ni}_{0.11})_3$ was arc melted, annealed at 1200°C (100 hr) in an argon-filled, fused silica capsule and then crushed into powder. X-ray powder patterns were taken with a Guinier-de Wolff focusing camera and a 114.6 mm diameter Debye-Scherrer camera ($\text{Cu } K\alpha$ radiation) with the asymmetrical film setting. The lattice constants were determined by the least-squares refinement of high angle diffraction data ($\lambda K\alpha_1 = 1.54051$ Å). The intensity calculations were made by the use of a Fortran IV program written by Jeitschko & Parthé (1966).

The diffraction pattern could be indexed with a 7-layered hexagonal unit cell having

$$a = 5.491 \pm 0.003, \quad c/a = 2.8538;$$

$$c = 15.67 \pm 0.01 \text{ \AA}; \quad V = 14.61 \text{ \AA}^3 \text{ per atom.}$$

In analogy with the well known structural principle (see e.g. Beck, 1968) for the TiNi_3 and TiPt_3 structures, it appeared likely that the $\text{Ti}(\text{Pt}_{0.89}\text{Ni}_{0.11})_3$ structure consists of identical, close packed ordered AB_3 layers which are similar to those found in close packed planes of the AuCu_3 structure.† These layers are stacked in the [001] direction such that there are no $A\text{-}A$ contacts and the coordination is twelvefold throughout. The possibility of ordered AB_3 layers having rectangular ordering as found in close packed planes of the SbCu_3 structure was also considered. However, structures derived from 'rectangular' layers are usually characterized by an orthorhombic distortion which was not found in the present structure.

With 'triangular' layers, the following stacking sequences for a 7-layered structure are possible (Beck, 1967): $52T$, $4\bar{1}11T$ and $3\bar{1}2\bar{1}T$.‡ Intensity calculations were made for each of these, assuming random distribution of Pt and Ni atoms on the B sites. Good agreement between the observed and calculated intensities (Table 1) could be obtained only with the stacking sequence $5\bar{2}T$. The layer stack-

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† These layers may be considered as having triangular ordering (Beck, 1968), or a T -type mesh.

‡ In the presently used stacking symbol (Zhdanov, 1945) alternating positive and negative integer numbers characterize the stacking sequence. They give the numbers of positive (e.g. in $a^+b^+c^+a^+b^+c^+$...) and negative (e.g. in $c^-b^-a^-c^-b^-a^-$...) stacking sequences; thus $5\bar{2}$ means five positive sequences followed by two negative ones in one period. T denotes the triangular intralayer ordering.

ing is $\dot{a}cab\dot{c}ab\dot{c}$, which is 28.6% hexagonal (stacking - $ihrrrrh$, where r denotes cubic stacking and h , hexagonal). The structure belongs to the trigonal system, space group $P\bar{3}m1$. The space group identification was facilitated by the use of Patterson-Kasper Tables (Patterson & Kasper, 1959). Assuming the origin to be at the center of symmetry within the first layer, the following atomic positions are obtained:

$$\text{Ti: } 1 (a): 0, 0, 0.$$

$$2 (c): \pm(0, 0, z); \quad z \approx \frac{2}{7}.$$

$$2 (d), 2 (d'): \pm(\frac{1}{3}, \frac{2}{3}, z); \quad z \approx \frac{4}{7}.$$

$$(\text{Pt}_{0.89}\text{Ni}_{0.11}): 3 (e): \frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; \frac{1}{2}, \frac{1}{2}, 0.$$

$$6 (i): \pm(x, \bar{x}, z); x, 2x, z; 2\bar{x}, \bar{x}, z);$$

$$x = \frac{1}{2}, z \approx \frac{2}{7}.$$

$$6 (i'), 6 (i''): \pm(x, \bar{x}, z); x, 2x, z; 2\bar{x}, \bar{x}, z);$$

$$x \approx \frac{1}{8}, z \approx \frac{3}{7}, \frac{5}{7}.$$

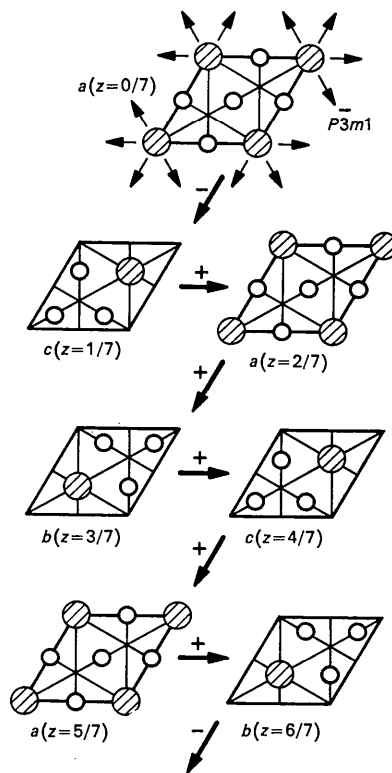


Fig. 1. The 7-layer stacking arrangement, $\dot{a}^-c^+a^+b^+c^+a^+b^-$, of triangularly ordered close packed AB_3 layers, which constitutes a unit cell of the $\text{Ti}(\text{Pt}_{0.89}\text{Ni}_{0.11})_3$ structure.

The positional parameters have been assigned idealized values for the close packing of equal-sized spheres. There is some justification for such a procedure, because of the fact that the interlayer separation, $c/7a$, is close to 0.40825, the value for close packing of equal-sized spheres.

Table 1. X-ray data for ordered Ti (Pt_{0.89}Ni_{0.11})₃
P $\bar{3}m1$; $a=5.491$, $c=15.67$ Å; Cu $K\alpha$ radiation.

hkl	$\sin^2 \theta \times 10^3$		I_{obs}	I_{calc}^* $\frac{52}{T}$ structure
	obs.	calc.		
001	—	2.4	—	0.0
002	—	9.7	—	0.0
003	—	21.8	—	0.0
100	26.1	26.3	vw	1.5
101	28.6	28.7	vw	2.8
102	35.8	36.0	w	21.9
004	—	38.7	—	0.0
103	48.0	48.1	vw	17.7
005	—	60.5	—	0.0
104	64.6	65.0	vw	12.2
110	79.1	78.8	m	19.0
111	—	81.3	—	0.0
105	86.2	86.8	vw	7.3
006	—	87.1	—	0.0
112	—	88.5	—	0.0
113	—	100.6	—	0.0
200	105.7	105.1	w	5.3
201	107.9	107.5	w	10.9
106	—	113.4	—	0.5
202	115.2	114.8	s	100.0
114	—	117.6	—	0.0
007	118.9	118.6	s	72.8
203	127.3	126.9	s	98.7
115	—	139.3	—	0.0
204	143.6	143.8	s	81.8
107	—	144.9	—	0.3
008	—	154.9	—	0.0
205	165.7	165.6	m	57.6
116	—	166.0	—	0.0
108	—	181.2	—	0.2
210	—	184.0	—	0.2
211	—	186.4	—	0.5
206 } 212 }	193.8	{ 192.2 193.6	vw	{ 4.5 4.7
009		—		196.0
117	197.5	197.4	m	10.3
213	206.2	205.7	vw	4.8
109 } 214 }	222.2	{ 222.3 222.7	vw	{ 1.9 4.3
207		223.9		223.7
118	—	233.7	—	0.0
300	236.7	236.5	vw	3.9
301	—	238.9	—	0.0
0,0,10	—	242.0	—	0.0
215	—	244.5	—	3.2
302	—	246.2	—	0.0
303	—	258.3	—	0.0
208	—	260.0	—	2.8
1,0,10	—	268.3	—	1.6
216	—	271.1	—	0.2
119	—	274.9	—	0.0
304	—	275.2	—	0.0
0,0,11	—	292.8	—	0.0
305	—	297.0	—	0.0
209	301.1	301.1	m	22.0
217	—	302.5	—	0.2

Table 1 (cont.)

hkl	$\sin^2 \theta \times 10^3$		I_{obs}	I_{calc}^* $\frac{52}{T}$ structure
	obs.	calc.		
220	315.7	315.4	ms	46.7
221	—	317.8	—	0.0
1,0,11	—	319.1	—	1.2
1,1,10	—	320.9	—	0.0
306	—	323.6	—	0.0
222	—	325.0	—	0.0
223	—	337.1	—	0.0
218	—	338.8	—	0.2
310	—	341.6	—	0.1
311	—	344.1	—	0.2
2,0,10	347.8	347.1	w	19.9
0,0,12	—	348.5	—	0.0
312	—	351.3	—	1.8
224	—	354.1	—	0.0
307	355.8	355.1	vw	4.1
313	—	363.4	—	2.0
1,1,11	—	371.7	—	0.0
1,0,12	—	374.8	—	0.8
225	—	375.9	—	0.0
219 } 314 }	379.9	{ 380.0 380.4	vw	{ 1.6 1.9
308		—		391.4
2,0,11	397.9	398.0	m	16.2
315	—	402.1	—	1.5
226	—	402.5	—	0.0
0,0,13	—	409.0	—	0.0
400	—	420.5	—	0.6
401	—	422.9	—	1.3
2,1,10	—	426.0	—	1.6
1,1,12	—	427.3	—	0.0
316	—	428.8	—	0.1
402	430.5	430.2	w	12.6
309	—	432.5	—	0.0
227	433.3	433.9	ms	57.2
1,0,13	—	435.3	—	0.1

* The intensity listed for each set of indices $hk(i)l$ consists of the contribution from the corresponding reflection plus that of the reflection $h(i)kl$ which, though it has in general a different structure factor, superimposes with $hk(i)l$ on the powder diagram.

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