arc melted and then heat treated in an evacuated quartz tube for about two months at 450 °C. Because the alloy is slowly oxidized by air, fragments were sealed in thin pyrex capillaries for X-ray examination. Using Mo $K\alpha$ X-rays $(\lambda = 0.7107 \text{ Å})$ and a precession camera, the crystals were found to be hexagonal with $a = 9.92 \pm 0.02$ and $c = 6.33 \pm 0.02$ Å. With two Ce₇Ni₃ per unit cell the calculated density is 7.12 g.cm.-3, and the measured density of the gross alloy was 7.12 g.cm.⁻³. Reflections of type *hhl* with l = 2n + 1 were systematically absent. Thus the space group is $P6_3mc$, $P\overline{6}2c$ or $P6_3/mmc$. For intensity data, sets of timed exposures for each of the levels h0l, hhl and h1l were made with a precession camera and Mo $K\alpha$ radiation. Intensities were estimated visually by comparison with a series of spots of known relative intensity. Lp corrections (Waser, 1951) were computed with an IBM 704. No absorption corrections were made.

Considerations of atomic volumes had indicated that the most likely formula of the compound was Ce_7Ni_3 . An hol Patterson projection was computed. Inspection of this Patterson quickly showed that the space group could not be $P6_3/mmc$, and a tentative structure was deduced by using space group $P6_3mc$. It was then realized that the compound is isostructural with the Th_7M_3 compounds described by Florio *et al.* (1956).

The structure was refined by least-squares using an IBM-704. Separate scale factors for each of the three reciprocal lattice levels and individual isotropic temperature factors were used as parameters in addition to the position parameters. The full matrix was used to determine parameter shifts and standard deviations. Form factors were used in functional form with the parameters given by Forsyth & Wells (1959). $P6_3mc$ is a polar space group, thus the value of one z parameter is arbitrary. The z of Ce₂ was, therefore, held fixed at zero. The results of the least-squares calculations are given in Table 1. These values may be compared with those of Florio et al. by adding $\frac{1}{4}$ to the present z parameters. The list of observed and calculated structure factors is given in Table 2. With unobserved reflections omitted, the overall value of R is 9.1%. For the levels h0l, hhl and hll, R is respectively 7.7, 9.1 and 11.7%.

The interatomic distances are given in Table 3. The atoms listed are those which satisfy the definition of a neighbor given by Frank & Kasper (1958). The Ni atom has nine Ce neighbors forming a polyhedron with 14 three-sided faces. The six closest atoms are at the corners of a distorted trigonal prism, and the other three atoms lie outward from the rectangular faces of this prism. Each Ce atom has 15 neighbors. Ce₁ has three Ni and 12 Ce neighbors which form a polyhedron with 26 three-sided

Table 3. Interatomic distances in Ce₇Ni_a

The numerals in parentheses denote the number of crystallographically equivalent distances. The standard deviation of these distances is about 0.025 Å.

Co Ni	(9)	9.09 \$	Co Ni	(0)	0.00 1
00_1 – M	(3)	2.92 A	Ce_3-NI	(2)	2.83 A
$-Ce_2$	(3)	3.82	–Ni	(2)	3.53
$-Ce_3$	(3)	3.54	-Ce,	• •	3.54
$-Ce_3$	(3)	3 ·79	-Ce,		3.79
$-Ce_3$	(3)	3.91	-Ce ₁		3.91
Ū			-Ce ₂	(2)	3 ∙66
			–Ce,	(2)	3.77
Ce ₂ –Ni	(2)	2.87	-Ce ₃	(2)	3.44
–Ni		3.05	$-Ce_3$	(2)	3.80
–Ni		3.64	Ŭ	• •	
$-Ce_1$		3.82	Ni-Ce,		$2 \cdot 92$
$-Ce_2$	(2)	3.72	-Ce,	(2)	2.87
$-Ce_2$	(4)	3.82	–Ce,	. ,	3 ·05
$-Ce_3$	(2)	3 ∙66	$-Ce_2$		3.64
$-Ce_3$	(2)	3.77	$-Ce_3$	(2)	2.83
-			-Ce ₃	(2)	3.53

faces. Ce₃ has four Ni and 11 Ce neighbors also forming a polyhedron with 26 three-sided faces but different from that about Ce₁. Ce₂ has four Ni and 11 Ce neighbors which form a polyhedron having 22 three-sided faces and two four-sided faces. These polyhedra are outlined in Fig. 1. All of the edges of the convex polyhedra about the Ni atom and Ce₂ join common neighbors but this is not the case for Ce₁ and Ce₃.

In the paper by Florio *et al.* (1956), Table 1, which lists the interatomic distances in Th_7Fe_3 , is in error with respect to both the distance given and the identification of the neighbors. The neighbors in Th_7Fe_3 correspond with those given in our Table 3, and the actual distances, in most cases, differ by about 0.05 Å.

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References

- COFFINBERRY, A. S. (1960). Private communication.
- CROMER, D. T. & LARSON, A. C. (1959). Acta Cryst. 12, 855.
- CROMER, D. T. & OLSEN, C. E. (1959). Acta Cryst. 12, 689.
- FLORIO, J. V., BAENZIGER, N. C. & RUNDLE, R. E. (1956). Acta Cryst. 9, 367.
- FORSYTH, J. B. & WELLS, M. (1959). Acta Cryst. 12, 412.
- FRANK, F. C. & KASPER, J. S. (1958). Acta Cryst. 11, 184.
- VOGEL, R. (1947). Metallforschung, Stuttgart, 2, 97.
- WASER, J. (1951). Rev. Sci. Instrum. 22, 563.

Acta Cryst. (1961). 14, 1087

On the nature of the omega phase in quenched titanium alloys. By JU. A. BAGARJATSKIJ, G. I. NOSOVA and T. V. TAGUNOVA, Central Scientific Research Institute for Ferrous Metallurgy, 23 Radio Street, Moscow, USSR

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There was a time when the crystal structure of the omega phase in titanium alloys was the subject of some doubt (Silcock, Davies & Hardy, 1955; Bagarjatskij, Tagunova & Nosova, 1955; Yoshida, 1956; Austin & Doig, 1957; Spachner, 1958), but it has now been established (Bagarjatskij & Nosova, 1958; Silcock, 1958). The omega phase has a hexagonal lattice with c/a = 0.612-0.613 in Ti-base alloys (Silcock *et al.*, 1955; Bagarjatskij *et al.*, 1955; Bagarjatskij & Nosova, 1958; Silcock, 1958) or 0.622– 0.625 in Zr-base alloys (Hatt, Roberts & Williams, 1957; Anderko, 1959). For Ti-base alloys the space group is $P\overline{3m}1$ and the atomic positions 000, $\pm \frac{1}{3}\frac{2}{3}z$, with z =0.480–0.495 (Bagarjatskij & Nosova, 1958; Silcock, 1958).

There are many indications that a metastable omega phase appears on annealing quenched beta-phase alloys at temperatures not higher than 450-550 °C. (Brotzen, Harmon & Troiano, 1955; Bagarjatskij, Nosova & Tagunova, 1958; Holden & Young, 1958; etc.), but it has also been detected in many quenched titanium alloys (Silcock et al., 1955; Yoshida, 1956; Brotzen et al., 1955; Bagarjatskij, Tagunova & Nosova, 1958), although in restricted ranges of composition (Bagarjatskij, Nosova & Tagunova, 1958). We have found that in a Ti + 6% Cr alloy the omega phase forms on quenching from the beta region even at a quenching rate exceeding 5000 °C. per second. It is very doubtful if diffusion processes can occur during such drastic quenching. It has been noted earlier that in alloys with 8% Cr the omega phase can be formed from the beta phase by deformation (Bagarjatskij, Tagunova & Nosova, 1958), and that in alloys with 15% V the amount appearing after quenching can be increased by compressive deformation (Brotzen et al., 1955).



Fig. 1. The atomic arrangements in the beta phase (left, atomic plane $1\overline{10}$) and in the omega phase (right, atomic plane $11\overline{20}$). The directions of the displacements of rows of atoms in the beta-to-omega transformation are indicated. The magnitude of the displacement s is approximately one-sixth of the interatomic distance.

All these facts indicate that in some circumstances there is a diffusionless beta-to-omega transformation. The close relation of the crystal structures and the strict orientation relationship between the phases suggest that the transformation displacements are less than the interatomic distances (Fig. 1). The different electrical properties of the phases, in spite of the identity of composition (Brotzen *et al.*, 1955; Bagarjatskij, Tagunova & Nosova, 1958) suggest that the transformation occurs as a result of instability of the beta-phase electron structure at temperatures lower than 450-550 °C. (Bagarjatskij, Nosova & Tagunova, 1958). This may be similar to the beta-alpha transformation in brass (Jones, 1937).

The omega phase may thus be interpreted as a metastable low-temperature modification of the beta solid solution, and the phase change at high cooling rates as a transformation in a one-component system. There is an almost complete analogy with the martensitic transformation in the copper-base alloys Cu–Zn, Cu–Al and Cu–Sn (Kurdjumov, 1958). The difference is that in the latter the atomic displacements necessary for the formation of the martensitic structures $(\alpha', \beta', \beta'' \text{ or } \gamma')$ from the high-temperature β phase all have approximately the same direction, accounting for the visible relief on the specimen surface. In the beta-omega transformation, on the other hand, neighbouring rows of atoms are displaced in opposite directions (Fig. 1), and cannot cause surface relief.

The data available at present thus indicate that the omega transformation takes place in two ways: as a diffusion-controlled process during annealing, and as a diffusionless process during quenching or deformation of alloys containing rather less of the second element. This is similar to the formation of the α' phase (martensite) from austenite in iron-carbon alloys: the former appears either without diffusion during quenching, or by a diffusion-controlled process during the bainitic transformation.

The recently discovered inversion of the beta-omega transformation in Ti-Cr and Ti-Fe alloys at high rates of heating and cooling (Gridnev, Rafalovskij, Trefilov & Černenko, 1959; Gridnev, Petrov, Rafalovskij & Trefilov 1960) may also be considered as a confirmation of the martensitic nature of the omega phase.

Because of the absence of rolief after beta-omega transformation, it may be called a martensitic transformation of a special kind.

References

- ANDERKO, K. (1959). Z. Metallk. 50, 681.
- AUSTIN, A. E. & DOIG, J. R. (1957). J. Met. 9, 27.
- BAGARJATSKIJ, JU. A. & NOSOVA, G. I. (1958). Kristallografija, 3, 17.
- BAGARJATSKIJ, JU. A., NOSOVA, G. I. & TAGUNOVA, T. V. (1958). Dokl. Akad. Nauk SSSR, 122, 593.
- BAGARJATSKIJ, JU. A., TAGUNOVA, T. V. & NOSOVA, G. I. (1955). Dokl. Akad. Nauk SSSR, 105, 1225.
- BAGARJATSKIJ, JU. A., TAGUNOVA, T. V. & NOSOVA, G. I. (1958). Sbornik 'Problemy Metallovedenija i Fisiki Metallov', Moscow, 5, 210.
- BROTZEN, F. R., HARMON, E. L. & TROIANO, A. R. (1955). J. Met. 7, 413.
- GRIDNEV, V. N., RAFALOVSKIJ, V. A., TREFILOV, V. I. & ČERNENKO, N. F. (1959). Voprosy Fisiki Metallov i Metallovedenija, 10, 77. Kiev.
- GRIDNEV, V. N., PETROV, JU. N., RAFALOVSKIJ, V. A. & TREFILOV, V. I. (1960). Voprosy Fisiki Metallov i Metallovedenija, 11, 82.
- HATT, B. A., ROBERTS, J. A. & WILLIAMS, G. J. (1957). Nature, Lond. 180, 1406.
- HOLDEN, F. C. & YOUNG, A. P. (1958). Trans. Metall. Soc. of AIME. 212, 287.
- JONES, H. (1937). Proc. Phys. Soc. 49, 250.
- KURDJUMOV, G. V. (1958). Žurnal Tekhničeskoj Fiziki, 18, 999.
- SILCOCK, J. M. (1958). Acta Met. 6, 481.
- SILCOCK, J. M., DAVIES, M. H. & HARDY, H. K. (1955). Nature, Lond. 175, 731.
- SPACHNER, S. A. (1958). Trans. Metall. Soc. of AIME. 212, 57.
- YOSHIDA, H. (1956). J. Jap. Inst. Metals. 20, 292.