SOVIET PHYSICS – SOLID STATE VOL. 12, NO. 2 AUGUST, 1970

PHASE TRANSFORMATION OF TITANIUM AND ZIRCONIUM IN SHOCK WAVES

V. N. German, A. A. Bakanova,
L. A. Tarasova, and Yu. N. Sumulov

Translated from Fizika Tverdogo Tela, Vol. 12, No. 2,
pp. 637–639, February, 1970
Original article submitted September 1969;
revision submitted October 7, 1969.

The metals of the IVa group of the periodic table – titanium and zirconium – have a hexagonal close-packed lattice (α phase) at normal temperatures and pressures. The high-temperature β phases of these metals have body-centered cubic lattices. The properties of titanium and zirconium at high pressures were first studied by Bridgman [1–3], who inferred in the abrupt changes in volume and resistance in titanium and zirconium the existence in them of a high-pressure phase. Jamieson [4] determined the structure of these phases by x-ray structural investigations under pressure. It was found that the high-pressure phases of these metals continue to exist after the pressure is relieved and have hexagonal lattices of a new type under normal conditions (with crystallographic constants of $a = 4.625$, $c = 2.813$ Å and $a = 5.036$, $c = 3.109$ Å for titanium and zirconium, respectively). Three atoms entering into the composition of the unit cell are found at lattice points with coordinates (0, 0, 0), (2/3, 1/3, 1/2), and 1/3, 2/3, 1/2). The high-pressure phase was called the ω phase. X-ray investigations performed by the authors [5] confirmed the presence in zirconium of an ω phase. Table 1 gives the constants of unit cells of the α, β, and ω phases of the metals studied.

We studied in the present investigations samples of titanium and zirconium subjected to short-term pulsed loading by shock waves with amplitudes of 120, 200, 350, and 500 kbar. The method of loading and preserving the samples is that of Al'tshuler et al. [6]. After the shock the titanium and zirconium samples underwent x-ray investigation on a URS-50 IM diffractometer.

The lines of a new phase were observed in zirconium samples for all shock-pressure amplitudes. The maximum amount of the new phase, which exceeded the content of the initial phase, was obtained at pressures of 350 kbar. Table 2 shows the results of calculating the interplanar distances of a zirconium sample under a pressure P = 350 kbar. Values of the interplanar distances of original zirconium according to Mirkin [7], interplanar distances and relative line intensities of the ω phase calculated from the data of Jamieson [4], and also interplanar distances and relative intensities for a lattice we shall discuss below are given in the table for comparison. The relative intensities were calculated taking into account the polarization, Lorentz, geometric (form), structure, and multiplicity factors.

TABLE 1. Parameters of Known Polymorphous Phases of Titanium and Zirconium

	α phase		ω phase		β phase*		New phase
	a, Å	c, Å	a, Å	c, Å	t, °C	a, Å	a, Å
Ti	2.95	4.69	4.625	2.813	882	3.28	3.276
Zr	3.23	5.14	5.036	3.109	862	3.59	3.568

Note. *Parameters of the β phase were determined by extrapolation of data obtained at high temperatures to normal temperatures.

TABLE 2. Values of the Interplanar Distances of Zirconium under a Pressure P = 350 kbar, and the Interplanar Distances of Its Modifications

Sample under pressure P = 350 kbar		Original structure [7]			Structure of the ω phase [4]			Structure of new phase		
d	I	d	hkl	I	d	hkl	I	d	hkl	I
—	—	—	—	—	3.103	001	6	—	—	—
2.794	med	2.798	010	33	—	—	—	—	—	—
2.568	med	2.573	002	33	—	—	—	—	—	—
—	—	—	—	—	2.533	011	45	—	—	—
2.523	v.s.	—	—	—	2.521	110	100	2.522	011	100
2.460	s.	2.459	011	100	—	—	—	—	—	—
—	—	—	—	—	1.957	111	13	—	—	—
1.897	w.	1.894	102	17	—	—	—	—	—	—
1.784	med.	—	—	—	1.786	021	20	1.783	002	22
1.615	w.	1.616	110	17	—	—	—	—	—	—
—	—	—	—	—	1.555	002	11	—	—	—
1.459	med.	1.463	013	18	1.455	121	50	1.457	112	54
1.395	v.w.	1.399	020	3	—	—	—	—	—	—
1.366	med.	1.368	112	18	—	—	—	—	—	—
1.350	w.	1.350	021	12	—	—	—	—	—	—
—	—	—	—	—	1.323	112	43	—	—	—
—	—	—	—	—	1.317	031	3	—	—	—
1.285	v.w.	1.287	004	4	—	—	—	—	—	—
1.260	med.	—	—	—	1.259	220	19	1.262	022	19
1.228	v.w.	1.229	022	4	—	—	—	—	—	—
1.127	med.	—	—	—	1.129	131	14	1.128	013	32
1.0858	v.w.	1.0842	023	4	—	—	—	—	—	—
—	—	—	—	—	1.062	032	14	—	—	—
1.0351	w.	1.0360	121	6	1.037	003	1	—	—	—
1.029	med.	—	—	—	1.029	041	7	1.029	222	1
—	—	—	—	—	1.008	013	15	—	—	—
0.9783	w.	0.9783	123	2	0.9784	222	15	—	—	—
0.9534	s.	—	—	—	0.9525	231	13	0.9534	123	60
—	—	—	—	—	0.9517	140	15	—	—	—

Note. We use the following notation: d are the interplanar distances; hk*l* are the Miller indices; I is the intensity; v.s. is very strong; s is strong; med. is medium; w. is weak; v.w. is very weak.

As the table shows the new high-pressure phase we obtained in zirconium after a shock wave has passed through it is not the ω phase of [4]. This is indicated by the absence on x-ray diffraction photographs of the ten comparatively strong lines of the ω phase, and also the lack of correspondence of experimental and calculated intensities. The indexing of seven lines of the new phase showed that all of them correspond with great precision to a lattice with the structure of a body-centered cube with a = 3.568 ± 0.005 Å. The density of the new phase ρ = 6.656 g/cm^3.

A high-pressure phase was also identified in titanium, but only in samples subjected to a pressure p = 350 kbar. On the x-ray diffraction photographs of these samples three new, not very strong lines are present. The absence of lines of a new phase in titanium samples subjected to a pressure P = 500 kbar, and their low-intensity in zirconium samples for the same pressures are apparently explained by their instability at the high residual temperatures of shock compression. Just as in zirconium, these lines can be ascribed to the strongest reflections from (011), (002), and (022) of a cubic phase with a = 3.27 Å. Unfortunately, these lines coincide with (110), (021), and (220) of the titanium ω phase. The absence of other strong reflections of the ω phase compels us to presume that we succeeded in isolating the body-centered cubic high-pressure phase in titanium, as in zirconium.

The last column of Table 1 shows the parameters of the new metastable phases of Zr and Ti; they were, however, obtained at much lower temperatures.

LITERATURE CITED

1. P. W. Bridgman, Proc. Am. Acad. Arts Sci., 76, 71 (1948).
2. P. W. Bridgman, Proc. Am. Acad. Arts Sci., 81, 165 (1952).
3. P. W. Bridgman, Proc. Am. Acad. Arts Sci., 76, 55 (1948).
4. J. C. Jamieson, Science, 3 (3562), 72 (1963).
5. A. Gayaraman, W. Klement, and G. G. Kennedy, Phys. Rev., 131, 644 (1963).
6. V. L. Al'tshuler, I. M. Barkalov, I. N. Dulin, V. N. Zubarev, T. N. Ignatovich, and P. A. Yampol'skii, Khimiya Vysokikh Energii, 2, 88 (1968).
7. L. I. Mirkin, Handbook of X-ray Structural Analysis [in Russian], GIFML, Moscow (1961).