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B1-type and WC-type phase bulk bodies of tantalum nitride prepared by shock and static compressions

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Abstract

Tantalum nitride (TaN) is a unique nitride which has CoSn-type structure at ambient state among the transition metal nitrides (1 : 1). We have been performing the shock- and static-high-pressure compression experiments to synthesize the dense-phase tantalum nitrides. The single-phase bulk body of B1-type tantalum nitride with good stoichiometry was prepared by shock compression. The single-phase bulk bodies of B1- and WC-type tantalum nitrides were also prepared by static compression. The static-compression quenching experiments showed that the B1-type phase was a high-temperature high-pressure phase and the WC-type phase was a low-temperature high-pressure phase. The B1- and WC-type phases bulk bodies had good high-temperature stabilities and much higher hardnesses than the CoSn-type. The shock-compression-synthesized B1-type one showed superconductivity with a comparatively high critical temperature.

Keywords: Tantalum nitride; High-pressure phase; Shock compression; Static compression; Superconductivity

1. Introduction

Tantalum nitride (TaN) is a unique nitride which has CoSn-type structure at ambient state among the transition metal nitrides (1:1) [1]. The tantalum nitride dense phases of WC- and B1-type are expected to have high hardness, and the latter one is theoretically predicted to have high superconducting critical temperature [2]. The B1-type phase tantalum nitride materials have been synthesized by means of various methods [3–9]. However, the materials prepared by these methods were mixtures with other compounds such as Ta_2N or nonstoichiometric B1-type phase. In addition, the bulk materials of the B1-type phase cannot be prepared, except by high-pressure methods. The WC-type phase tantalum nitride material was so far synthesized only by the static compression, while the chemical composition was nonstoichiometric [3].

We have been performing the shock-compression recovery and static-compression quenching experiments to synthesize the dense-phase tantalum nitrides. We succeeded in the preparation of the single-phase bulk bodies of B1- and WC-type tantalum nitrides with good stoichiometry by shock and static compressions [10–12]. We have been investigating the physical properties of these dense phases. In this report, the synthesis experiments are reviewed, and some physical properties are shown.

2. Synthesis by shock compression

Almost all the single-phase bulk body of B1-type tantalum nitride was prepared by shock compression of the CoSn-type phase porous material [10].

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Table 1
Crystal and chemical data of the CoSn-type [10], WC-type [11] and B1-type [10] phases of tantalum nitride

Phase	CoSn-type	WC-type	B1-type
Synthesis method	Combustion	Static compression	Shock compression
Structure	Hexagonal	Hexagonal	Cubic
	B35, P6/mmm	Bh, P6m2	B1, Fm3m
Lattice parameters	$a_0 = 0.51923 + (1)$	$a_0 = 0.2934 + (2)$	$a_0 = 0.43363 + (1)$ nm
	$c_0 = 0.29083 + (1)$	$c_0 = 0.2880 + (2)$ nm	
Composition	$TaN_{0.97-1.00}$	$TaN_{1.04}$	$TaN_{0.96-0.99}$
Properties, etc.	Ambient phase	Low-temperature high-pressure phase	High-temperature high-pressure phase
		High-hardness	High-hardness
			Super conductivity

Shock-compression recovery experiments were conducted using a powder gun [13], using the porous samples of 13, 55 and 70% in porosity in the impact velocity range of 1.2–1.5 km/s. The recovery rate of the B1-type phase depended strongly on the porosity rate, and almost 100% recovery rate was achieved for the shot using a 70% porosity and with an impact velocity of faster than 1.4 km/s (tungsten impactor of 2 mm in thickness). It was confirmed that the nitrogen content did not change by shock compression. The chemical formula of the shock-compression synthesized B1-type phase was estimated to be $TaN_{0.96-0.99}$, while combustion-synthesized ones to be $TaN_{1.13-1.30}$. The X-ray density of the shock-compression synthesized B1-type phase was calculated to be 15.9 g/cm^3, which was denser than that of the CoSn-type phase ($TaN_{0.99}$) of 14.3 g/cm^3. The crystal and chemical analytical data of the B1-type phase synthesized by shock compression are summarized in Table 1.

3. Synthesis by static compression

Almost all the single-phase bulk bodies of both of WC- and B1-type phases were prepared by static compression of the CoSn-type phase powder [11]. The quenching experiments under static compression in the pressure range of up to 3 GPa and in the temperature range of 1000–1800°C were performed on the CoSn-type tantalum nitride, using a piston-cylinder-type apparatus. The WC- and B1-type phases were recovered from the high-pressure conditions of 0.8–3 GPa at lower than 1500–1800°C and at higher than about 1800°C, respectively. This indicated that the B1-type phase was a high-temperature high-pressure phase and the WC-type phase was a low-temperature high-pressure phase, respectively. The B1- and WC-type phases maintained a good stoichiometry. The X-ray density of the static-compression synthesized B1-type ($TaN_{0.99}$) and WC-type phase ($TaN_{1.04}$) were calculated to be 15.9 and 15.1 g/cm^3, respectively. The crystal and chemical analytical data of the WC-type phase synthesized by static compression are also summarized in Table 1.

4. Some physical properties of the B1- and WC-type phase tantalum nitrides

Some physical properties of the B1- and WC-type phase materials were investigated. The Vickers hardness of the B1-type phase bulk body prepared by shock compression increased substantially with the transformation rate [12]. This suggested that the B1-type phase had much higher hardness than the CoSn-type one. The hardnesses of the WC-type ones prepared by static compression were also much higher than the CoSn-type. As a result of the temperature treatment tests, the B1- and WC-type phases did not change under about 900°C and 1200°C [14], respectively. These results indicate that the B1- and WC-type phases showed good high-temperature stability. If the well-sintered

B1- and WC-type phase bulk bodies are prepared, new harder materials are expected to be developed.

We performed the resistivity and susceptibility measurements on the CoSn-type, WC- and B1-type phases tantalum nitrides. The B1-type phase bulk bodies prepared by shock compression showed superconductivity with the critical temperature of 7.4–9 K, while the CoSn- and WC-types did not show above 4 K. The high critical temperature of the B1-type bulk bodies, which is comparable to or higher than those of the sputtered films [4–7], may be due to the good crystal state and stoichiometry.

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