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Compression behavior of $VC_{0.85}$ up to 53 GPa

H.P. Liermann [a,*], A.K. Singh [b], B. Manoun [a], S.K. Saxena [a], V.B. Prakapenka [c], G. Shen [c]

[a] Center for the Study of Matter at Extreme Conditions (CeSMEC), Florida International University, 11200 SW 8th Street, Building VH 140, Miami, FL 33199, USA

[b] Materials Science Division, National Aerospace Laboratories, Bangalore, India

[c] Center for Advanced Radiation Sources, University of Chicago, Chicago, IL, USA

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Abstract

Samples of $VC_{0.85}$ sandwiched between aluminum disks were compressed in a diamond anvil cell and X-ray diffraction patterns recorded at high pressures up to 53 GPa using synchrotron radiation. The presence of aluminum in the cell rendered the sample pressure nearly hydrostatic and also served as the pressure standard. No phase transformation was observed up to the highest pressure. The measured unit cell volume versus pressure data gave 258 ± 11 GPa and 4.5 ± 0.6 for the bulk modulus and the pressure derivative, respectively.

Keywords: Vanadium carbide; Compressibility; Elastic properties; Bulk modulus

1. Introduction

Transition metal carbides show unique combination of properties such as, high-melting temperature, high hardness, good high-temperature strength, and good electrical and thermal conductivity. Hence carbides have long been used as high-temperature structural materials in the form of hard constituents in metal matrix composites or coatings on cutting tools [1–5]. VC_x in particular has been used as an additive to inhibit grain growth in WC during sintering [6–9]. These applications require a good understanding of the mechanical properties of the carbides. The elastic properties have been measured both on polycrystalline sintered compacts and single crystals [10–13]. In the present study we have measured unit cell volume of V_8C_7 under high pressure and determined the bulk modulus and pressure derivative.

2. Sample preparation and experimental technique

Vanadium carbide powder of nominal composition V_8C_7 (Atlantic Equipment Engineers, purity 99.8%) was used in the present study. Vanadium and carbon contents were estimated by electron probe microanalysis. Carbon content was also estimated using Leco carbon analyzer with tungsten carbide standard. Fig. 1 shows the diamond anvil cell and the sample assembly used in the high-pressure experiments. The VC_x sample sandwiched between two high purity (99.999%) 15 μm thick aluminum disks was placed in the 200 μm hole in the rhenium gasket. X-ray diffraction patterns were recorded on an image plate using 10 μm incident X-ray beam ($\lambda = 0.3311$ Å) at the beamline ID13BM from the synchrotron source APS at the Argonne National Laboratory, Chicago.

3. Results and discussion

The results of microprobe analysis are shown in Table 1. These data suggest the composition of the sample as $VC_{0.85}$. This composition was also confirmed by direct carbon estimation. This composition implies a vacancy concentration of 2.9% with respect to the

* Corresponding author. Tel.: +1-305-348-3039; fax: +1-305-348-3070.
E-mail address: liermann@fiu.edu (H.P. Liermann).

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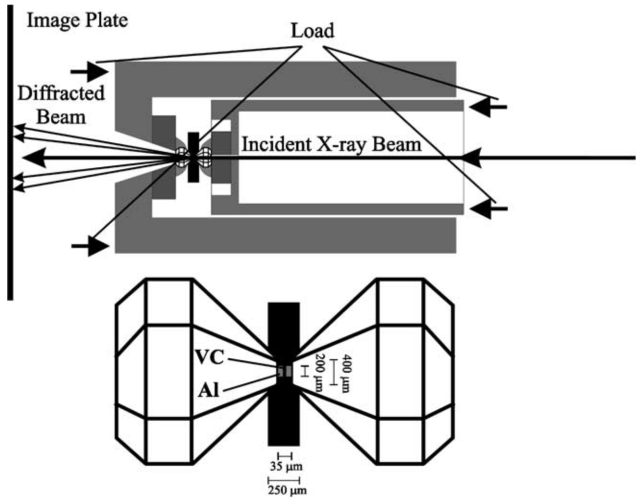

Fig. 1. Schematic illustration of the diamond anvil cell. Inset shows details of the sample assembly.

Table 1
Electron microprobe analysis of $VC_{0.85}$

Atom%	Analysis 1	Analysis 2
C	45.8378	46.0882
Fe	0.0000	0.0212
Pt	0.0948	0.0116
Au	0.0637	0.0305
Co	0.0194	0.0059
Cu	0.0000	0.0000
Ag	0.0033	0.0000
Ni	0.0254	0.0000
V	53.9347	53.8405
Nb	0.0000	0.0021
Ta	0.0210	0.0000
Total	100.0000	100.0000
C/*V*	0.849	0.856

structure of V_8C_7. The X-ray diffraction pattern at ambient pressure (Fig. 2) could be indexed as ordered V_8C_7 structure [14]. The absence of broad peak between the reflections (2 1 1) and (2 2 2) indicates the absence of vacancy ordering [15].

The stress state of the sample compressed in a DAC can become highly nonhydrostatic if the sample material is hard and has low compressibility like VC. It has been shown in the past that the sample pressure can be rendered nearly hydrostatic by using large volume of low shear strength material as the pressure-transmitting medium. For example, using NaCl as the pressure-transmitting medium and also as a pressure standard the compressibility of SiC has been measured [16]. Unlike NaCl, Al does not undergo pressure-induced phase transition and the pressure–volume relation is well established [17]. These factors dictated the choice of Al as the pressure standard in the present experiments. The low shear modulus of Al also makes it a good pressure-transmitting medium.

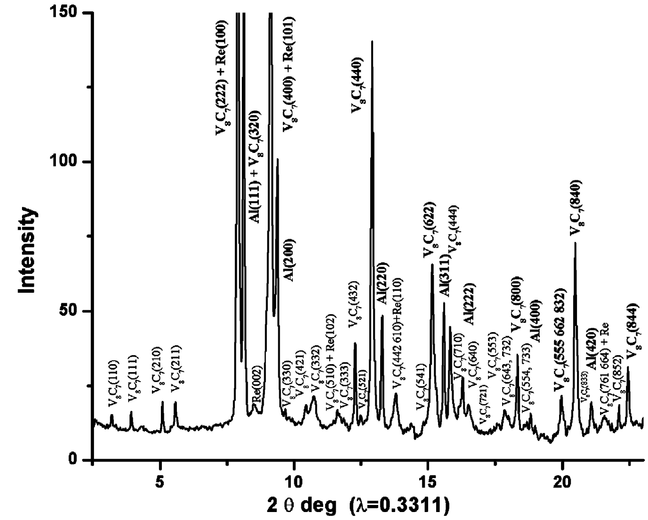

Fig. 2. X-ray diffraction pattern of $VC_{0.85}$ and Al at 1 bar in the diamond anvil cell.

Fig. 3 shows the typical quality of diffraction patterns as the pressure is increased. Because of the low diffraction angles and low intensities of the (1 1 0), (1 1 1), (2 1 0) and (2 1 1) reflections, only (2 2 2), (4 0 0), (4 4 0), (6 2 2), (4 4 4), (8 0 0), (6 6 2), and (8 4 0) reflections of $VC_{0.85}$ were considered in each run for determining the unit cell parameter. The (1 1 1), (2 0 0), (2 2 0), (3 1 1), (2 2 2) and (3 1 1) reflections from Al were considered. The diffraction angles were determined by fitting the four-parameter pseudo-Voigt function to each diffraction peak. The average lattice parameter and the standard error at each pressure were derived from the lattice parameters calculated from each reflection. The unit cell volume Al in each run was used to compute the pressure

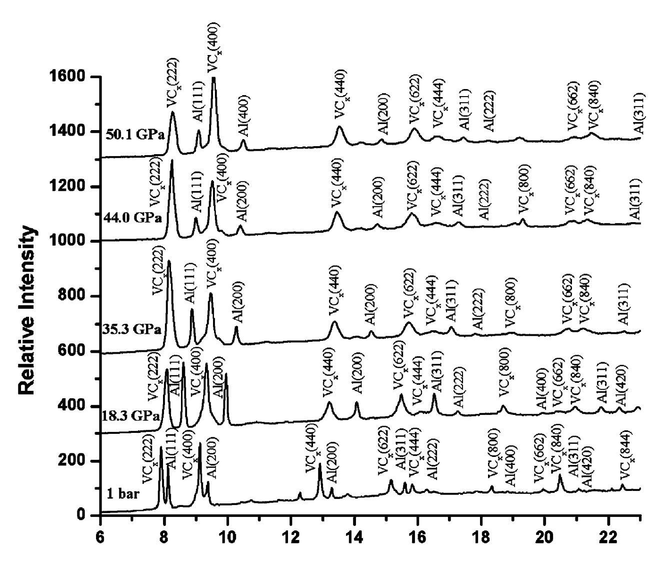

Fig. 3. X-ray diffraction pattern of $VC_{0.85}$ and Al at selected pressures between 1 bar and 50.3 GPa in the diamond anvil cell.

using $K_0 = 72.7$ GPa and $K_0' = 4.31$ for Al proposed earlier [16]. The pressure–volume data of $VC_{0.85}$ are shown in Table 2 and plotted in Fig. 4.

The pressure–volume relation for solids is known to fit two-parameter Birch–Murnaghan equation:

$$P = \frac{3}{2}K_0(x^{-7/3} - x^{-5/3})\left[1 + \frac{3}{4}(K_0' - 4)(x^{-2/3} - 1)\right].$$

K_0 and K_0' are the zero-pressure bulk modulus and first pressure derivative of the bulk modulus zero pressure, respectively. $x = V/V_0$, where V_0 and V are the unit cell volumes at zero pressure and high pressure, respectively. The Birch–Murnaghan fit to these data gives $K_0 = 258 \pm 11$ GPa and $K_0' = 4.5 \pm 0.6$ for $VC_{0.85}$.

The presence of vacancies in the structure is generally expected to reduce the elastic moduli. The measurement of single crystal elastic moduli by Brillouin scattering [13] indicates that while C_{11} of $VC_{0.88}$ (for V_8C_7, $x = 0.875$) is ~4% higher than the value for $VC_{0.84}$ but C_{12} and C_{44} remain practically unchanged for the two compositions. The bulk moduli calculated from these values for C_{11} and C_{12} are 246 ± 4 and 238 ± 4 GPa for $VC_{0.88}$ and $VC_{0.84}$, respectively. This suggests a value of 240 ± 4 GPa for the bulk modulus of $VC_{0.85}$. The present value of the bulk modulus is marginally higher than the combined error of the present and Brillouin scattering measurements.

Table 2
Unit cell volume data of $VC_{0.85}$ and Al, and pressures calculated Al-cell volumes

Run	V/V_0 ($VC_{0.85}$)	V/V_0 (Al)	P_{Al} (GPa)
vc-al-08-p00	1.0000(7)	1.0000(5)	0.01(1)
vc-al-08-p02	0.937(2)	0.8404(5)	18.4(1)
vc-al-08-p03	0.922(1)	0.8034(8)	25.5(2)
vc-al-08-p04	0.914(3)	0.787(1)	29.1(2)
vc-al-08-p05	0.909(3)	0.7789(6)	31.2(2)
vc-al-08-p06	0.895(2)	0.7630(9)	35.2(2)
vc-al-08-p07	0.887(4)	0.7454(6)	40.3(2)
vc-al-08-p08	0.886(3)	0.7408(5)	41.7(2)
vc-al-08-p09	0.881(3)	0.7343(8)	43.8(3)
vc-al-08-p10	0.874(3)	0.7257(6)	46.7(2)
vc-al-08-p11	0.871(2)	0.7222(8)	47.9(3)
vc-al-08-p12	0.869(2)	0.719(2)	49.1(8)
vc-al-08-p13	0.868(1)	0.7160(7)	50.1(2)
vc-al-08-p14	0.867(3)	0.7153(8)	50.3(3)
vc-al-08-p15	0.867(2)	0.708(3)	53(1)

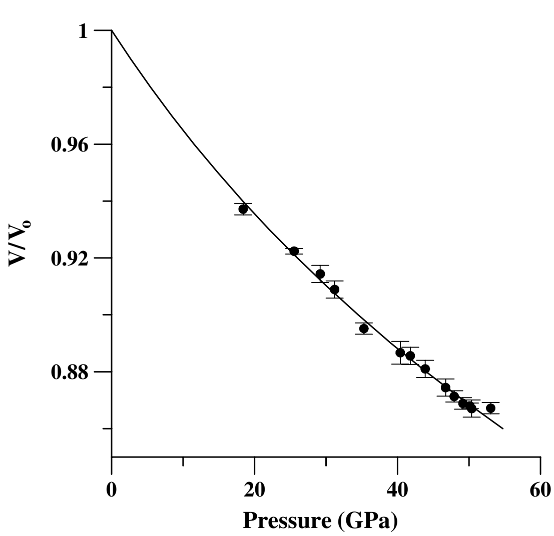

Fig. 4. Fit of Birch–Murnaghan equation to pressure volume data of $VC_{0.85}$.

4. Conclusion

The unit cell volume of $VC_{0.85}$ has been measured as a function of pressure up to 53 GPa. The pressure–volume data give 258 ± 11 GPa and 4.5 ± 0.6 for the zero-pressure bulk modulus and pressure derivative of the bulk modulus at zero pressure, respectively. The present value of the zero-pressure bulk modulus is marginally higher than the Brillouin scattering measurements (238 ± 4 GPa) at ambient pressure. No phase transition is observed up to 53 GPa.

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